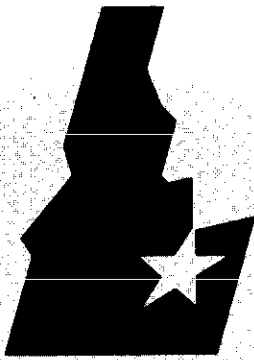


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**Idaho
National
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Laboratory**

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Department
of Energy*

Selection of Groundwater Flow and Contaminant-Transport Models for the Test Reactor Area at the Idaho National Engineering Laboratory



*Work performed under
DOE Contract
No. DE-AC07-76ID01570*

**Selection of Groundwater Flow and
Contaminant-Transport Models for the
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Published June 1992

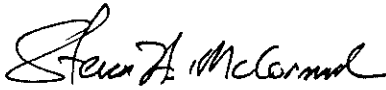
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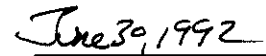
Selection of Groundwater Flow and Contaminant-Transport Models for the Test Reactor Area at the Idaho National Engineering Laboratory

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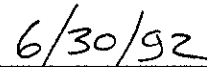
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ABSTRACT

This document provides background information to select groundwater flow and contaminant-transport models that can be used at the Idaho National Engineering Laboratory Test Reactor Area. These modeling activities will be used to simulate the migration of contaminants from the warm waste pond at the Test Reactor Area into the subsurface.

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ACRONYMS

CERCLA	Comprehensive Environmental Response, Compensation and Liability Act
CFA	Central Facilities Area
COCA	Consent Order and Compliance Agreement
CWP	cold waste pond
DOE	U.S. Department of Energy
DOE-ID	U.S. Department of Energy Idaho Field Office
EPA	U.S. Environmental Protection Agency
ChWP	chemical waste pond
ICPP	Idaho Chemical Processing Plant
INEL	Idaho National Engineering Laboratory
NPL	National Priorities List
RB	retention basin
RI/FS	remedial investigation/feasibility study
RWMC	Radioactive Waste Management Complex
SRPA	Snake River Plain Aquifer
STP	sewage treatment pond
TRA	Test Reactor Area
WWP	warm waste pond

Selection of Groundwater Flow and Contaminant-Transport Models for the Test Reactor Area at the Idaho National Engineering Laboratory

1. INTRODUCTION

This document discusses background information to select groundwater flow and contaminant-transport models that may be applied to the Test Reactor Area (TRA) at the Idaho National Energy Laboratory (INEL). The modeling activities simulate the migration of contaminants from the warm waste pond (WWP) into the subsurface.

The primary mission of the INEL is to support the engineering and operations efforts of U.S. Department of Energy (DOE) and other Federal agencies in the area of nuclear safety research, reactor development, reactor operations and training, nuclear defense material production, waste management and technology development, and energy conservation programs. Since 1952, the INEL has also been used as a storage facility for transuranic (TRU) waste and low-level waste.

The INEL was placed on the National Priorities List (NPL) under the Comprehensive Environmental Response, Compensation and Liability Act (CERCLA) in November 1989. The primary driving force for listing the INEL on the NPL was the WWP, which was also identified as a release unit under the Consent Order and Compliance Agreement (COCA) in July 1987. Therefore, the U.S. Department of Energy's Idaho Field Office (DOE-ID) initiated response planning at the WWP under CERCLA authorities. Following this, the Perched Water System remedial investigation/feasibility study (RI/FS) is being conducted at the TRA. Part of the RI/FS is a groundwater flow and contaminated-transport modeling study.

This document discusses the following items: (1) general site conditions, (2) model-selection criteria, (3) model data requirements and data availability, and (4) the advantages and disadvantages of recommended models.

1.1 Site Location and General Site Conditions

The INEL site is located 32 miles west of Idaho Falls, Idaho and occupies 890 square miles of the northwestern portion of the Eastern Snake River Plain (Figure 1). The INEL site is bound on the northwest by three major mountain ranges: Lost River, Lemhi, and Bitterroot (Figure 2). The INEL land surface is relatively flat, and predominant relief in the area is from volcanic vents (i.e., buttes) and unevenly surfaced and fissured basalt flows.

The climate at the INEL site can be characterized as semiarid with generally hot summers and cold winters. The temperature varies between a minimum of -40°F in January and 100°F in July, with a mean annual temperature of 44°F. The average precipitation at the INEL site is a relatively low

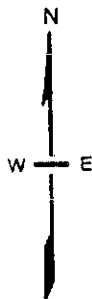
EXPLANATION



IDAHO NATIONAL
ENGINEERING LABORATORY

APPROXIMATE BOUNDARY OF
THE EASTERN SNAKE
RIVER PLAIN

GENERALIZED GROUNDWATER
FLOW LINE (MUNDORFF ET AL., 1964)



0 10 20 40 MILES

0 15 30 60 KILOMETERS

SCALE

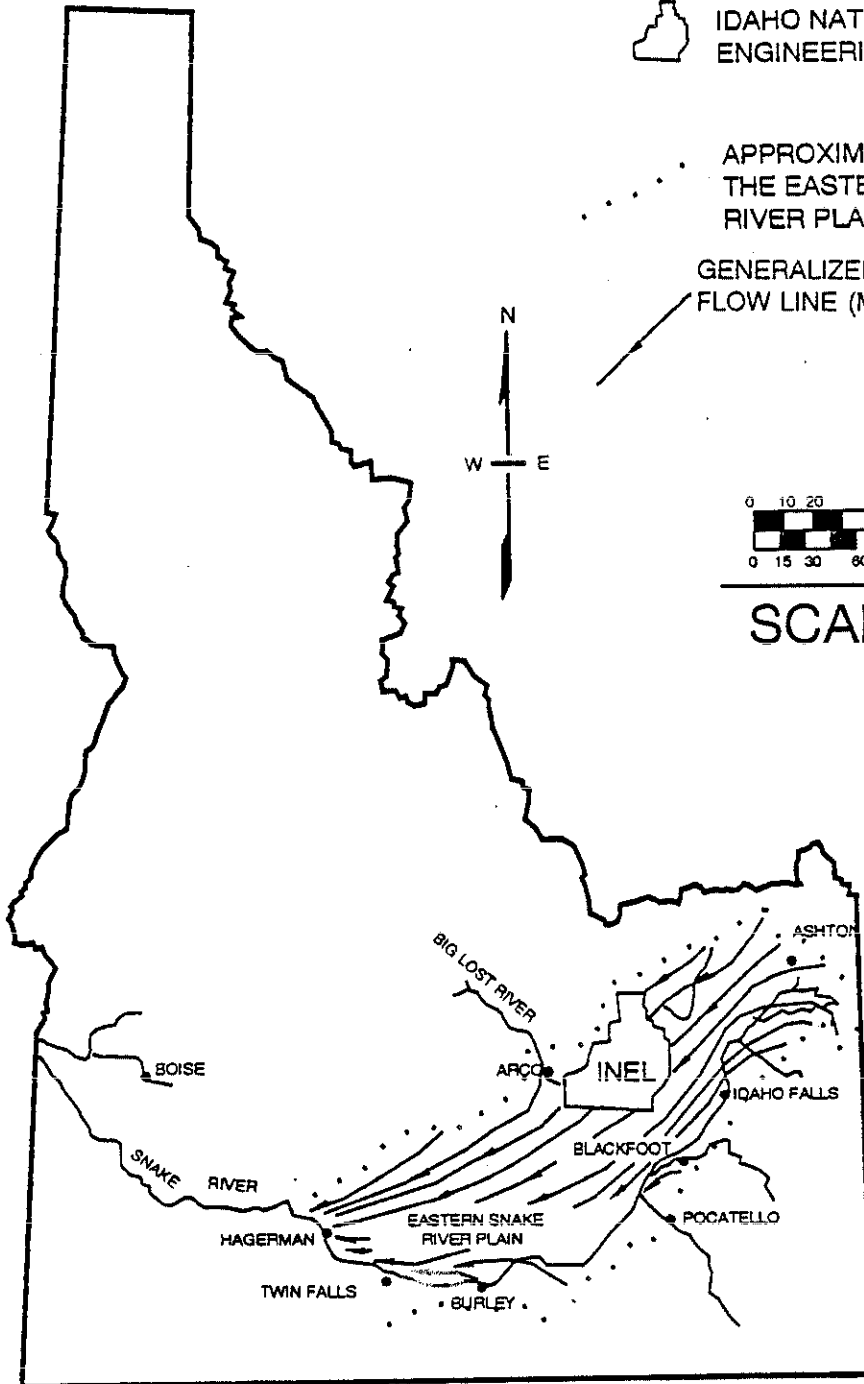
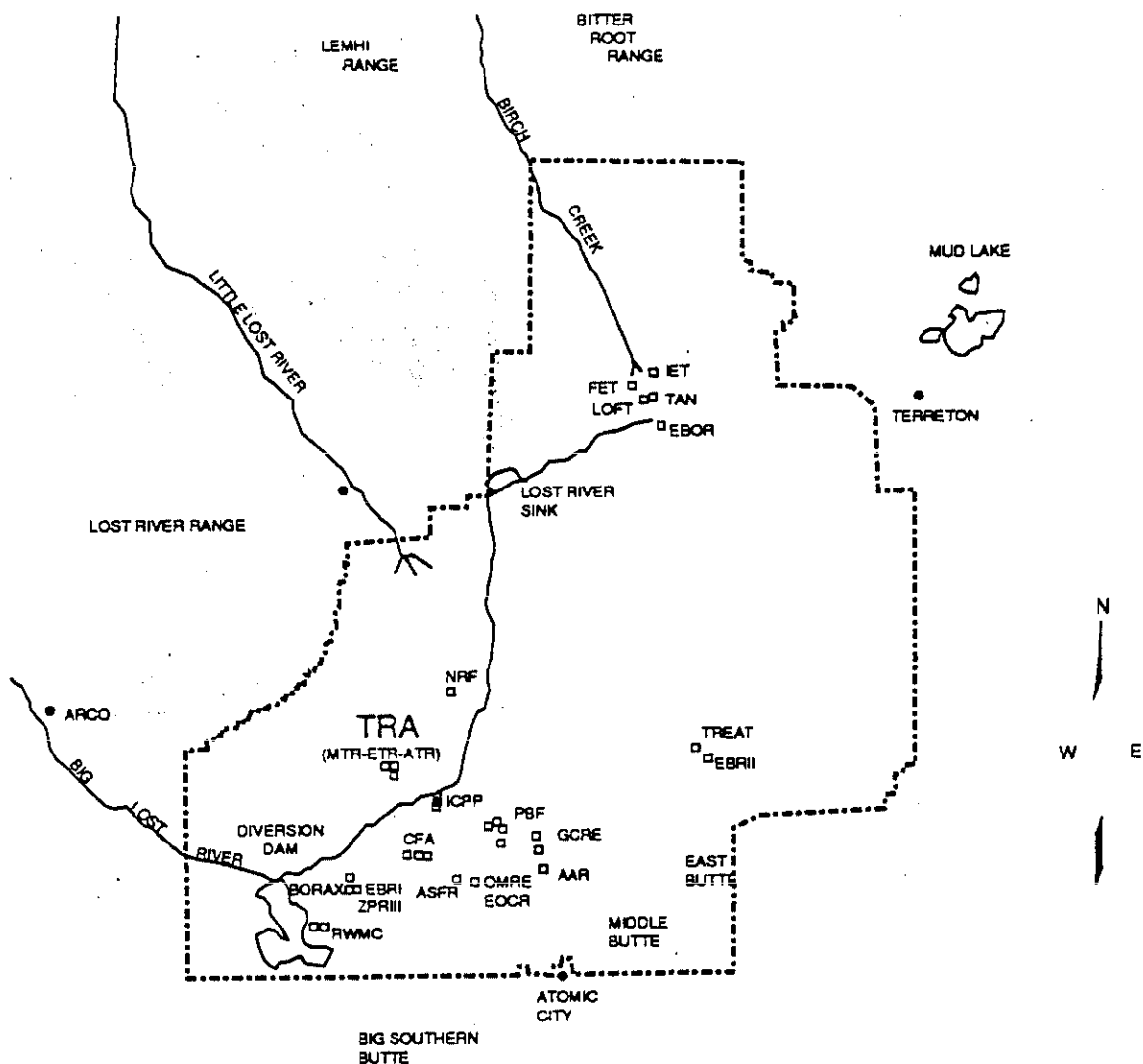


Figure 1. Map of Idaho Showing the location of the INEL, Snake River Plain, and generalized groundwater flow lines of the Snake River Plain Aquifer.



Name	Abbreviation
------	--------------

Advanced Test Reactor	ATR
Argonne Fast Source Reactor	AFSR
Army Reactor Area	ARA
Boiling Water Reactor Experiment	BORAX
Central Facilities Area	CFA
Engineering Test Reactor	ETR
Experimental Beryllium Oxide Reactor	EBOR
Experimental Breeder Reactor No. 1	EBR-I
Experimental Breeder Reactor No. 2	EBR-II
Experimental Organic Cooled Reactor	ECOR
Field Engineering Test Facility	FET
Gas Cooled Reactor Experiment	GCRC
Idaho Chemical Processing Facility	ICPP
Initial Engineering Test Facility	IET
Loss of Fluid Test Facility	LOFT
Materials Testing Reactor	MTR
Naval Reactors Facility	NRF
Organic Moderated Reactor Experiment	OMRE
Special Power Excursion Reactor Test	PBF
Test Area North	TAN
Test Reactor Area	TRA
Transient Reactor Test Facility	TREAT
Zero-Power Reactor No. 3	ZPR-III
Radioactive Waste Management Complex	RWMC

EXPLANATION

----- INEL BOUNDARY

□ FACILITIES

• TOWNS

0 2 4 6 8 10 MILES

SCALE

Figure 2. Location of the facilities within the INEL.

(9.09 in./yr) because most of the moisture is lost over the mountains to the north (Bowman et al. 1984). The monthly average relative humidity varies between 15% in August and 81% in the months of December to February (EG&G Idaho 1981).

Potential annual evaporation from saturated ground surface at the INEL site is approximately 36 in./yr, 80% of which occurs in the period of May through October. During the warmest month (July) the potential evaporation rate is around 0.25 in./day; whereas, during the coldest months (December through February) the potential evaporation rate is very low. However, the actual evaporation rate is much lower because the ground surface at the Site is usually not saturated. The evapotranspiration by native vegetation is estimated to be 6 to 9 in./yr (Linsley et al. 1982).

The TRA is located in the southwestern portion of the INEL site (Figure 2), with the Big Lost River curving around the Site to the south and east. The facility houses high neutron-flux nuclear test reactors. Wastewater associated with various waste streams are currently disposed in a series of unlined infiltration ponds (Figure 3). The wastewater consists of reactor cooling water, radioactive wastewater, laboratory waste, regeneration solutions from ion exchange columns and sanitary sewage treatment. Wastewater disposal has occurred on-Site since 1952.

1.2 Purpose and Scope

This document provides guidance for the selection of appropriate groundwater flow and contaminant-transport models for use at the TRA site. The selection process focuses on models appropriate for simulation of density coupled, variably-saturated flow and transport. This preselection is made because, as is described in Section 2, the area of interest is partly unsaturated and the concentration of some of the disposed contaminants is relatively high, which could require density-coupled flow modeling.

The selection process is based on criteria developed by the U.S. Environmental Protection Agency (EPA) for model evaluation (Bond and Hwang 1988). The model selection documentation is preceded by a description of the hydrogeologic and contaminant conditions at the site.

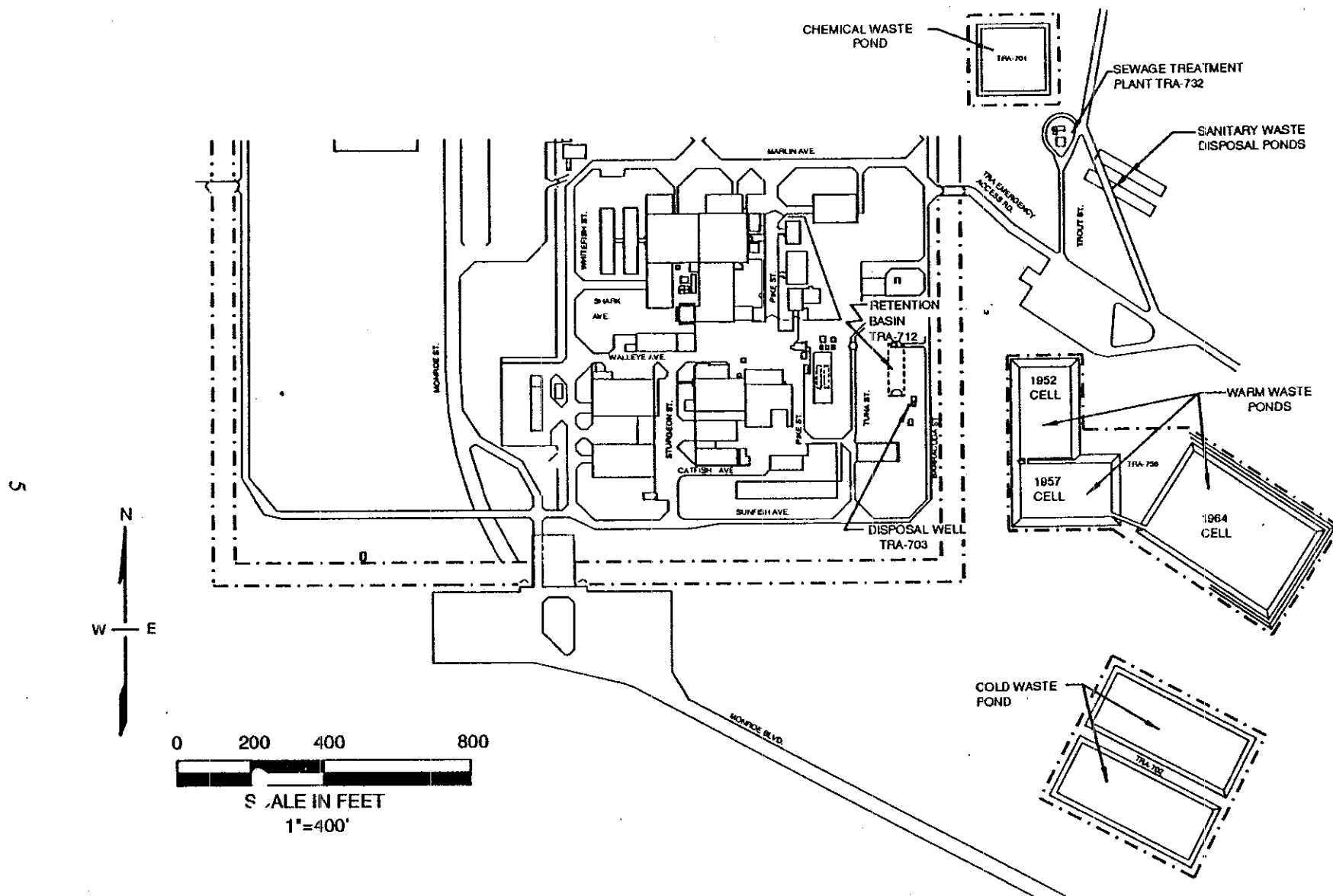


Figure 3. Map of the Test Reactor Area showing the location of the warm waste pond, retention basin, and disposal well.

2. GENERAL OVERVIEW OF THE HYDROGEOLOGIC AND CONTAMINANT SITE CONDITIONS

This section discusses the hydrogeologic conditions and the sources and characteristics of the contaminants at the TRA.

2.1 Hydrogeologic Framework

This section describes the hydrogeologic conditions at the TRA site in terms of the different water-bearing zones, lithology, and material properties.

There are three water-bearing zones of concern at the TRA. The shallowest zone is a small perched water zone in the surficial alluvium immediately under and adjacent to the disposal ponds at a depth of approximately 49 ft. Below that zone is a second perched water zone that has formed above a small-permeability layer that lies within the basalt at a depth of about 150 ft below the land surface. This deeper perched water zone is much larger than the shallow zone. The shallow and the deep perched groundwater zones exist because of the large volumes of water discharged into the disposal ponds (Langford 1971). The regional aquifer, the Snake River Plain aquifer (SRPA), is the third water bearing zone and occurs at a depth of approximately 450 ft below the ground surface. A generalized geologic cross section is shown in Figure 4.

2.1.1 Surface Alluvium

Beneath the WWP is approximately 45 to 55 ft of alluvial sediments deposited by the Big Lost River (Figure 4). The upper 35 to 50 ft generally consist of poorly sorted gravels, gravelly sands and sands with some fine grained materials. This is underlain in places by approximately 5 ft of clayey sands, sandy silt, and sandy clay materials that directly overlie the basalt or fill the basalt fractures (Mattick and Doornbos 1990). The bulk density for this layer varies from around 2.0 g/c for the top to around 1.55 g/c for the bottom although high values can also occur throughout the alluvium. The porosity varies from around 25% at the top to around 40% near the bottom, again a lower value can occur near the bottom. The hydraulic conductivity ranges from approximately 1 to 10 ft/d for the top of the layer and increases to 10^3 ft/d towards the bottom; although lower values of the order of 10 ft/d can be found near the bottom (Hull 1989).

2.1.2 Basalts and Interbeds

Beneath the alluvial sediments lie approximately 2,000 ft of basalt and interbedded sedimentary units (interbeds). The uppermost basalt unit, approximately 90 ft thick, extends to a depth of approximately 150 ft. The permeability of the basalt is highly variable and scale dependent because of the spatial distribution of fractures and lava tubes. Robertson (1977) used a value of 10 ft/d for hydraulic conductivity to model the deep perched water zone at the TRA. He also suggested that an average porosity of 10% is reasonable. Approximately 150 ft below land surface there is a 50 ft thick layer of silt; this silt layer probably forms the base of the deeper perched water zone (Figure 4).

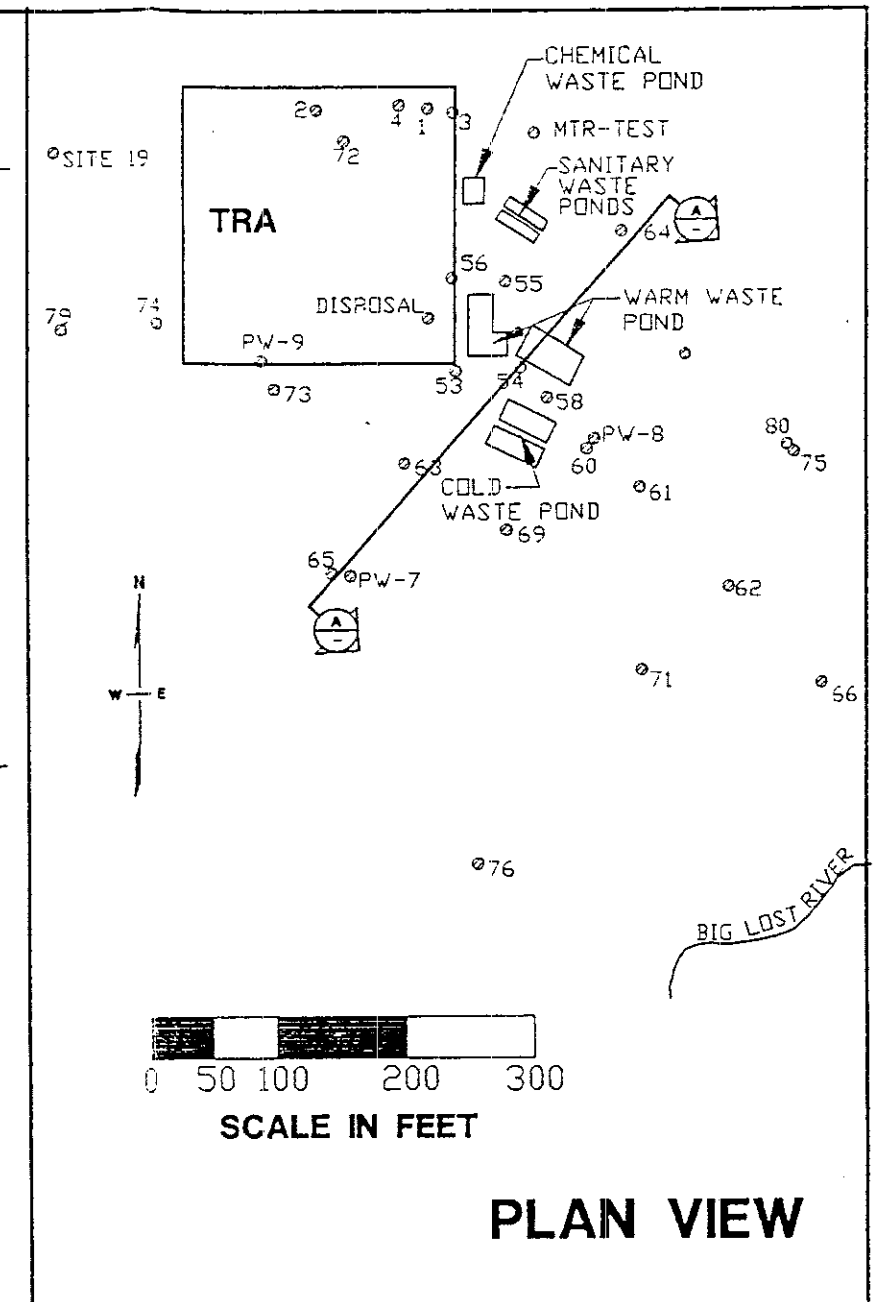
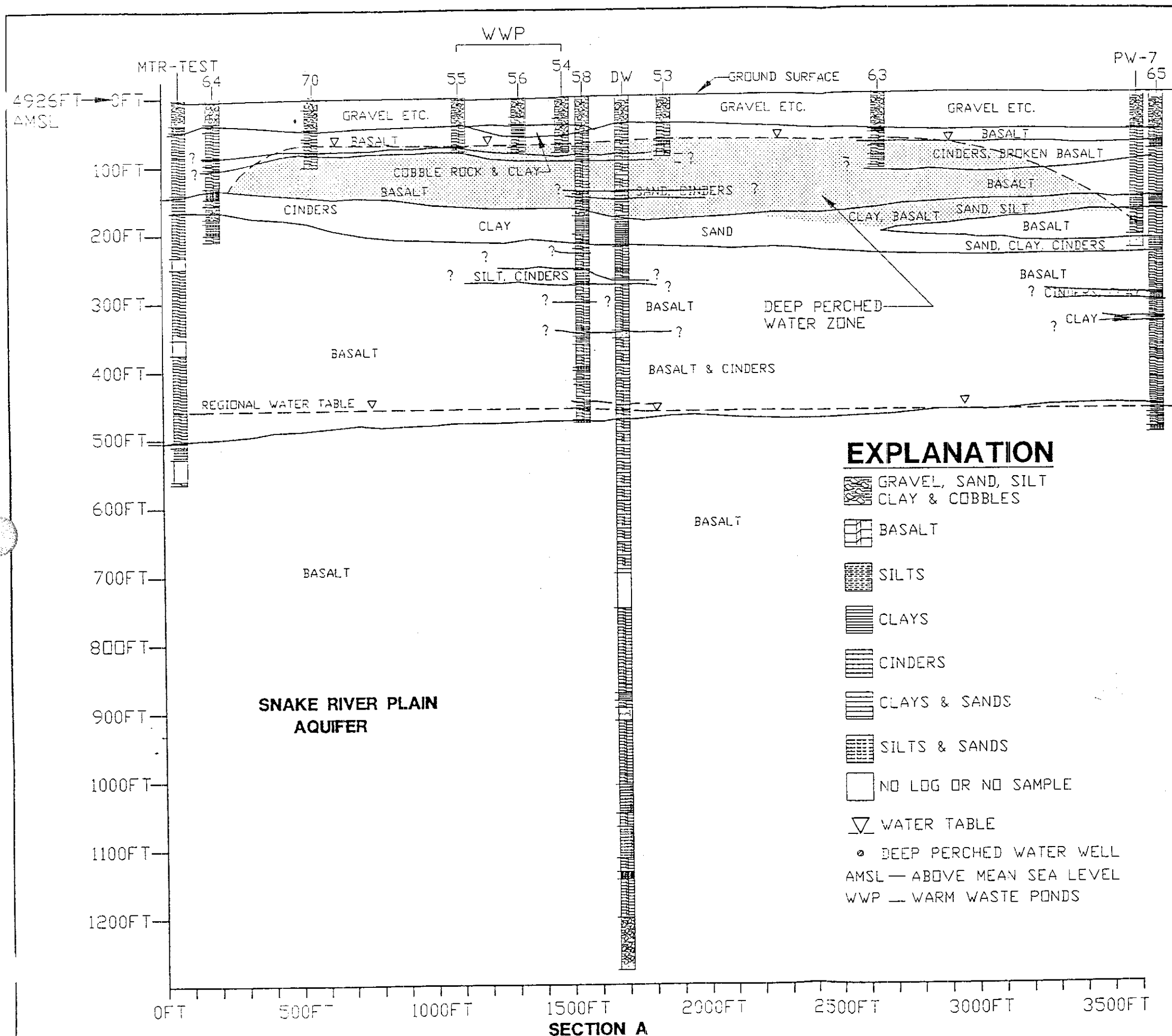


Figure 4. Geological cross section.

The materials below the deep perched water zone are a total of approximately 300 ft thick and consist of a composite of approximately 75 ft of sediment layers greater than 3 ft thick, approximately 220 ft of basalt and an estimated minimum composite thickness of 5 ft of sediment layers less than 3 ft thick (Robertson 1977). The interbed beneath the deep perched water zone is about 60 ft thick and is divided into two thinner layers to the south (Figure 4). This interbed will be referred to as the 150-ft interbed. There are generally at least two additional thinner interbeds beneath the 150-ft interbed. The layers have generally been observed to be mixed clays, silts, sands and gravels and are, on the average, considerably finer grained than the surface alluvial sand and gravel layer. Little data are available for materials below the 150-ft interbed and Robertson (1977) indicates that vertical hydraulic conductivity, based on soil analyses, has a median value of approximately 7×10^{-2} ft/d, and an arithmetic mean of 1 ft/d. The effective overall vertical hydraulic conductivity, based on modeling results (Robertson, et al. 1974), lies closer to the harmonic mean of 1.1×10^{-5} ft/d. The hydraulic properties for basalt beneath the 150-ft interbed would have to be assumed to be similar to those in the interval between the surface alluvium and the deep perched water body (Robertson 1977).

2.1.3 Snake River Plain Aquifer

The SRPA consists of a series of saturated basalt flows and interlayered pyroclastic and sedimentary beds (Figure 4). The SRPA is approximately 200 miles long, 40 to 60 miles wide and covers an area of 9,600 square miles (Figure 1). The lateral extent of the SRPA are defined by the contacts of the SRPA with the less permeable rocks at the margins of the plain (Mundorf et al. 1964). The effective thickness of the SRPA is considered to be the upper 250 ft of the basalt below the regional water table (Hull 1989). Aquifer permeability is controlled by the distribution of highly-fractured basalt flow tops and interflow zones, with some additional permeability contributed by vesicles and intergranular pore spaces.

Transmissivity of the SRPA at the TRA is estimated at approximately 16 million gal/d/ft. This probably represents a local high-transmissivity zone of approximately 12 square miles in the area (Walton 1958). A more reasonable estimate for southern INEL would be around 2.2 million gal/d/ft (Hull 1989). Beneath the TRA site the average water table gradient is approximately 2 ft/mi (Lewis and Goldstein 1982).

The storage coefficients are relatively high (0.02 to 0.06). The effective porosity estimates range from 5 to 15%, with 10% being the most accepted value (Robertson et al. 1974). The porosity estimate is a spatial average over a large volume because the aquifer is composed of massive basalt with a porosity of only a few percent and fractures and cinder zones with very high porosity (Hull 1989). Estimates of the total amount of water in storage in the SRPA vary between 2 billion acre-ft (Robertson et al. 1974) and 400 million acre-ft (Barracough 1989). Groundwater pumped for irrigation from the SRPA totals about 1.6 million acre-ft/yr (Hackett et al. 1986).

Three wells (TRA 1, TRA 3, and TRA 4) in the northeast corner of TRA supply water for TRA operations including drinking water. These wells are completed in and withdraw water from the regional aquifers. Production rates in 1964 were almost 3 million gal/d (Hull 1989). More recent data have not yet been found. Other production wells that are downgradient (with respect to the regional aquifer) from the TRA are two wells at the Central Facilities Area (CFA) (Figure 2), the Experimental Breeder Reactor 1 well, the firing range well, the rest-stop well on Highway 20/26, and the production well at the Radioactive Waste Management Complex (RWMC) (Hull 1989).

2.2 Recharge

Recharge occurs at the Site in the form of infiltration from wastewater disposal ponds and in the form of infiltration of precipitation, irrigation water and underflow from valleys adjacent to the Snake River Plain, and recharge because of leakage from the Big Lost River. Wastewater is discharged to the following infiltration ponds at the TRA (Figure 2).

- WWP
- TRA disposal well
- Chemical waste pond (ChWP)
- Sewage treatment pond (STP)
- Cold waste pond (CWP)
- USGS Well 53.

A description of the types and origin of contaminants emanating from the infiltration ponds and injection wells is given in Section 2.4.

2.2.1 Warm Waste Pond

The WWP system consists of a retention basin (RB) (concrete tank) from which the waste is led to the actual WWP via a pipe line. The RB has two concrete tanks, each of which has a 360,000 gallon capacity, and are used to allow radionuclides with short half-lives to decay before entering the WWP. A leak was identified in the RB in 1970, but it is not known when the leak started. It is estimated that the leakage rate is 86,000 gpd (325,510 L/day) when the two RB cells are used and 69,500 gpd (263,058 L/day) when only the west cell is used (Langford 1971).

A leak in the pipeline between the RB and the WWP was discovered in August 1963. Morris et al. (1963) concluded from measurements, that the basalt in the area of the leak stored between 1 1/2 to 4 years of discharge.

The WWP consists of three infiltration cells. The first cell was excavated in 1952. The second cell was added in 1957 when the capacity of the 1952 cell became too small because of reduced infiltration capacity and increased discharges. The two cells together have a capacity of 9.7 million gal (36.7 million L). During the early 1960s the infiltration capacity continued to decrease because of precipitation of salts and growth of algae on the bottom of the ponds. Therefore, cell 3 was excavated in 1964 with a capacity of 6.2 million gal (23.5 million L).

During the early 1950s the discharge was around 80 million gal/yr. This increased in 1956 and 1957 to about 100 million gal/yr. Between 1958 and 1978 the discharge varied between 125 million gal/yr and 283 million gal/yr with an average of 210.8 million gal/yr. From 1979 the discharge decreased to around 19 million gal/yr in 1987 with an average of 38.4 million gal/yr (Hull 1989).

The evaporation loss, when both of the 1952 and 1957 ponds were full, would have amounted to 1.3 to 1.5 million gal/day (Hull 1989).

2.2.2 TRA Disposal Well

The TRA disposal well is located 275 ft west of the WWP (Figure 3). The well was drilled in 1962 and 1963 and put into service in November 1964. The well is cased to a depth of 1,271 ft, with 1/4 in. x 6 in. slot perforations in the casing from 1,182 to 1,267 ft, from 930 to 1,070 ft, and from 512 to 697 ft (Hull 1989).

Discharge to the TRA disposal well increased from 90 million gal/yr in 1965 to 457 million gal/yr in 1976, with an average of 196.9 million gal/yr. From 1977 through 1981, the discharge varied between 244 million gal/yr and 382 million gal/yr (averaging 298.6 million gal/yr). In 1982, before the TRA disposal well ceased to be in use for disposal, 37 million gal were discharged. The TRA disposal well is now used as a monitoring well.

2.2.3 Chemical Waste Pond

The ChWP is located 750 ft north of the WWP (Figure 3) and was excavated in 1962 and first used in November of that year. The ChWP has a capacity of 3.2 million gal.

Discharge to the ChWP fluctuated around 45 million gal/yr from 1963 to 1971. The peak discharge was 73 million gal/yr in 1972; the discharge decreased from 31 million gal/yr in 1973 to 5.5 million gal/yr in 1987. The average annual discharge between 1963 and 1987 was 28.3 million gallons (Hull 1989).

2.2.4 Sewage Treatment Pond

The STP is located approximately 400 ft north of the WWP (Figure 3) and has been in use since 1952. The sewage treatment system is composed of a collection system, drainoff tank, trickling filter, chlorination basin, drying beds and two seepage ponds (i.e. the STP) in which the effluent finally is disposed. The estimated flow through the sewage system is 30,000 gpd (113,550 L/day). Records between 1984 and 1987 show an average annual discharge of 7.1 million gal to the STP.

2.2.5 Cold Waste Pond

The CWP was constructed in 1982 350 ft south of the WWP. The CWP has a capacity of 1,080,000 gpd (4,088,160 L/min), and the average annual discharge was 226.8 million gal between 1982 and 1987 (Hull 1989).

2.2.6 USGS Well 53

The USGS Well 53 was used between November 1960 and January 1962, June 1963 and August 1963, and November 1963 and September 1964 (Morris et al. 1965). This well is 90 ft deep and is located halfway between the TRA disposal well and the edge of the CWP. The injection rates were estimated at approximately 100 gpm (378.5 L/min).

2.2.7 Other Recharge

Recharge to the SRPA has a number of sources.

- Infiltration of irrigation water (5.1 million acre-ft/yr)
- Valley underflow (1.5 million acre-ft/yr)
- River seepage (1.3 million acre-ft/yr)
- Precipitation (0.8 million acre-ft/yr) (Hackett et al. 1986, Hull 1989).

Recharge to the SRPA from within INEL boundaries is primarily in the form of infiltration from the rivers and streams draining the areas to the north, northwest, and northeast of the Snake River Plain. The TRA waste disposal ponds contribute to the groundwater. In most years, spring snowmelt produces surface runoff that accumulates in depressions in the basalt or playa lakes (Hull 1989). On the INEL site, water not lost to evapotranspiration recharges the aquifer because the INEL site is within a closed topographic depression. Significant recharge from high flow in the Big Lost River causes a regional rise in the water table over much of INEL (some wells have shown a rise of as much as 6 ft) (Pittman et al. 1988).

2.3 Groundwater Movement

Past research has indicated that the groundwater in the Snake River Plain generally moves towards the south-southwest. However, local variations in the groundwater flow direction occur (Nace et al. 1956, Barraclough et al. 1981). Hull (1989), suggests conceptualizing the SRPA as a large porous medium where the individual grains are tens to hundreds of feet in diameter in order to get an understanding of the process of groundwater movement in the SRPA. The flow would then follow a sinuous path, around, through, and between the large particles in the general direction of the regional hydraulic gradient. The rate of the horizontal groundwater flow in the SRPA is estimated at 4.5 ft/d, based on an average transmissivity value of 2,210,000 gpd/ft a gradient of 3.8×10^{-4} ft/ft and an effective porosity of 10% (Hull 1989). VanDeusen and Trout (1990) concluded from calculations and measurements that the best estimate of the lateral ground water flow rate near the TRA is around 11 ft/day.

At the TRA disposal well, a downward groundwater flow potential exists, based on head measurements at depths of 590 ft and 1000 ft (Morris et al. 1965). Currently, no vertical hydraulic conductivity data exists so the quantities of vertical flow can not be estimated.

Travel times through the perched water system have been reported to be on the order of 1.5 to 2 years, with the majority of time taken up in getting to the lower basalt.^a On the other hand, extremely rapid travel times through an uninterrupted basalt flow (on the order of one month) have also been indicated.^a

a. Unpublished report by S. O. Magnuson, Idaho National Engineering Laboratory, EG&G Idaho, Inc., SOM-5-91, May 15, 1991.

2.4 Contaminant Source Characteristics

The contaminant source under investigation as part of the Perched Water Zone RI/FS is arising from the nonsanitary waste disposal at TRA. This section discusses the wastes going into the disposal units mentioned in Section 2.2 (see also Figure 3).

2.4.1 Warm Waste Pond

The following radionuclides have been discharged to the WWP:

- Tritium (as tritiated water)
- Chromium-51
- Cobalt-60
- Strontium-90
- Cesium-137.

Furthermore, before 1964, nonradioactive wastewater containing chromate was discharged to the pond. This chromium was used in the reactor cooling systems as a corrosion inhibitor. Before mid-1964, the TRA chemistry labs routinely discharged used chemicals and reagents into the WWP system. At the present time, warm wastewater exceeding a radioactivity of $1 \times 10^{-3} \mu\text{Ci/mL}$ is shipped to the Idaho Chemical Processing Plant (ICPP).

Measurements of the waste streams disposed in the WWP indicate that approximately 33,000 Ci were discharged to the pond between 1961 and 1985 (EG&G Idaho 1986). Radionuclides with relatively long half lives (30 years) are those were disposed in significant quantities (Hull 1989).

Because of the break in the pipeline feeding the WWP, it is likely that alluvial sediments became contaminated with the wastes found in the waste stream. The break was repaired in August 1963. The discharge monitoring showed that the leak probably existed for a number of years before identification (Morris et al. 1963).

2.4.2 TRA Disposal Well

The TRA disposal well was used primarily to dispose of cold liquid waste, including cooling tower blowdown water and water from air conditioning units, secondary system drains, and other nonradioactive drains. Before 1972 the hexavalent chromium concentrations were maintained at 10 to 14 mg/L (EG&G Idaho 1986); however, since 1972, phosphate-based corrosion inhibitors were used to replace the chromium. On one occasion, in 1981, a minor amount of radioactive primary cooling water was released into the well (VanDeusen & Trout 1990).

2.4.3 Chemical Waste Pond

The ChWP is used to dispose wastewater from ion exchange columns and water softeners. This water primarily contains sulfuric acid, sodium hydroxide and sodium chloride. This pond affects the perched water zones at the TRA and must be taken into consideration during the modeling activity.

From 1962 to mid-1984, it is estimated that the wastewater discharged to the ChWP contained 1.8×10^6 kg sodium hydroxide and 9.9×10^6 kg sulfuric acid. Since August 1984, regenerants have been routed through an existing brine tank where they are held until they can be neutralized before discharge to the pond. Significant quantities of dissolved salts are discharged into this pond; in 1987 244,944 kg of sulfate and 111,586 kg of sodium were disposed there.

2.4.4 Sewage Treatment Pond

The effluent to the STP has also been monitored since 1986 and the monitoring results showed that the sewage lagoons are not a source of contaminants to the Perched Water System (Environmental Monitoring, 1986, 1987, 1988).

2.4.5 Cold Waste Pond

After the TRA disposal well was taken out of service in 1982 the cold wastewater was rerouted to the CWP. The effluent has been monitored since 1986 and was characterized as relatively clean, according to the most current results (1988).

2.4.6 USGS Well 53

During the periods the USGS Well 53 received waste, the TRA disposal well was not yet in place and the third WWP well was not yet completed. It is believed that secondary coolant blowdown water (containing chromates) was discharged into this well although no data are available on types of waste and concentrations (Hull 1989).

3. MODEL SELECTION

This section discusses selection criteria, objectives and scope of the modeling study, describes relevant groundwater flow and contaminant-transport models, and recommends appropriate models for simulating Site conditions.

The term "model" in this report refers to computer codes that can be used to represent site hydrogeologic conditions and the subsurface movement of contaminants. The models incorporate Site-specific data, and interpretations of and estimates derived from Site-specific data, to represent the site. The combination of a computer code (model) and Site-specific data will be referred to in this report as a "Site-specific model."

3.1 Purpose and Scope of Modeling

The planned modeling activities provide a means by which project goals can be met. Specifically, the modeling activity will support and provide input into the feasibility and risk assessment studies. The overall modeling objectives are:

- To synthesize and interpret the Site-specific data into a coherent representation of the Site
- To provide a means by which ongoing field programs can be assessed and improved
- To predict future contaminant and groundwater flow conditions. Such predictions will be used to select and design potential remedial measures, and, to support risk assessment computations.

The current Perched Water System RI/FS data set and ongoing and planned field activities are adequate to proceed with the RI/FS modeling activities. The availability of data for modeling purposes is discussed in Section 4.

The following groundwater flow and transport modeling is planned. Initially, the modeling of the INEL will involve a two-dimensional variably saturated Site-specific model of the area below the WWP down to the SRPA, oriented along the local groundwater gradient in the SRPA. This two-dimensional Site-specific model will be used to develop a three-dimensional, variably saturated, Site-specific model. The three-dimensional model will be used to address feasibility-study and risk assessment objectives, and will incorporate all of the key processes and factors that affect the movement of contaminants in the subsurface.

3.2 Model-Selection Criteria

Selection criteria for groundwater flow and transport models fall into three categories (Bond and Hwang 1988): objectives criteria, technical criteria, and implementation criteria. These categories are discussed in the following sections.

3.2.1 Objectives Criteria

Objectives criteria are used to separate models into two groups: those that are designed for general or screening studies, and those that are designed for detailed studies. General or screening studies accomplish rapid, first-cut comparisons between sites for the purpose of ranking sites, and gain an understanding of the important factors at a particular site affecting transport and fate of contaminants. Such studies are often used when there are many sites to characterize or compare, or during the initial phases of field investigations when there are little field data available. Models that are appropriate for general or screening studies are analytical, compartmental, or very simple numerical models (one-dimensional, or simple two-dimensional models). Model data requirements are limited and predicted results should be regarded as preliminary and relative.

The purposes of detailed studies are to assess facility performance, environmental impact, and the performance of remedial solutions. Detailed studies are often used as field investigations progress and the quantity of available data increases in amount, complexity and variety. Appropriate models are most often numerical models, because they can incorporate complex heterogeneity, boundary conditions, a variety of specific contaminants, and the effects of multi-dimensional dispersion on transport. Numerical models are typically more difficult to develop, calibrate, maintain, and evaluate than analytical or compartmental models. The predicted results are generally more reliable and realistic than those from analytical or compartmental models.

There are two general categories of detailed studies: site-wide and local. Site-wide studies address issues that concern the entire site. These issues may include: (a) the estimated time required for a contaminant to migrate to the boundary of the site, (b) the concentrations that are likely to occur in groundwater if the contaminant reaches the site boundary, (c) the effect of conditions outside the site on the transport and fate of contaminants within the site (such as changes in groundwater recharge), and (d) the assessment of the relative importance of various parameters in controlling contaminant migration. Local studies address issues that concern individual sources or a subset of sources, including: (a) study of the factors that affect flow and transport in the vicinity of a waste-burial vault, (b) an assessment of remedial alternatives, (c) an assessment of the relative importance of various parameters that control contaminant migration, (d) the identification of probable contaminant sources, (e) the guidance of field programs and the assessment of the adequacy of the data for modeling, and (f) the evaluation of alternative conceptual models.

For the INEL site, detailed studies on a local and Site-wide basis are planned. General or screening models are not appropriate.

3.2.2 Technical Criteria

Technical criteria are used to select models that are capable of addressing the important technical issues. The selected model must be able to incorporate important mass transport and transformation processes, and to adequately simulate the important domain characteristics and material/fluid properties. The technical criteria must be applied within the context of the objectives criteria, and must consider the nature and extent of the existing data.

For contaminant-transport and transformation processes, the selected model must be able to incorporate the important factors that affect the transport of contaminants, such as advection and hydrodynamic dispersion. The selected model must also be able to simulate chemical processes that affect the concentration of a contaminant, such as decay, adsorption, or biodegradation.

In choosing the model domain configuration, the selected model must be adequately represent the physical system. Components of the physical system may include

- Confined and unconfined flow
- Horizontal and vertical flow
- Saturated and unsaturated conditions
- Variation in layer thicknesses
- Spatial distribution and temporal variations in boundary conditions (such as groundwater recharge, discharge, and pumpage)
- Spatial distribution and temporal variations in contaminant sources (such as point or areal sources, types of contaminants and concentrations).

All of these conditions occur to some extent at the INEL.

For fluid and material properties, the selected model must be able to incorporate relevant variations in material and fluid properties. These may include:

- Porous or fractured media
- Horizontal and vertical variations in material properties (such as hydraulic conductivity, and porosity)
- Single fluid, multi-fluid (multi-phase), or liquid and gas/vapor-phase flow
- Flow affected by density variations or temperature gradients.

For the TRA site, multiphase flow, temperature gradients, and vapor-phase flow are not important. The importance of density-coupled flow and transport may be evaluated as part of the Perched Water System RI/FS.

3.2.3 Implementation Criteria

After the objectives and technical criteria have been resolved, implementation criteria are used to select the final model or set of models. Implementation criteria address the following questions:

- Is the model available for review in the public domain or is it proprietary? Specifically, if a proprietary model is available to public agencies and non-profit organizations for evaluation and use, the model is considered to be "in the public domain."
- Is the model readily available and is the model well documented?
- Has the model been verified against analytical solutions or other previously verified models? Are the verification data sets available and well documented?
- Has the model been applied successfully at other sites (i.e., has the model been "field-tested")?

3.2.4 Site-Specific Model Selection Criteria

Based on the prior discussion of the various model-selection criteria, four specific selection criteria were developed:

- The selected model(s) must be capable of simulating conditions that exist at the TRA site. To satisfy this criteria, the selected model(s) should not require any more than minor modifications. Specifically, the selected model(s) should be able to incorporate:
 - Unconfined conditions
 - Two-dimensional vertical and three-dimensional flow
 - Saturated and unsaturated conditions
 - Porous media (fractures might need to be represented by a special porous layers or blocks)
 - Heterogeneous materials
 - Density coupled flow
 - Variation in layer thicknesses
 - Advection
 - Dispersion
 - Adsorption
 - Radioactive decay
 - Spatial distribution and temporal variations in boundary conditions. (Areal recharge, evapotranspiration, constant head, constant flux, and stream leakage)

- Spatial distribution and temporal variations in contaminant sources. (For the TRA site, the model(s) must be able to simulate areal sources, must allow the specification of initial contaminant concentrations, and must be able to simulate advection, dispersion, adsorption, and radioactive decay.)
- The selected model(s) must be able to satisfy the objectives of the study. The model(s) should be neither too simple, such that model results are unrealistic, nor too complex, requiring extensive input data that may be difficult to obtain. For the TRA site, the objectives are to:
 - Predict the magnitude and direction of fluid movement caused by wastewater discharge to the ponds and the retention basin
 - Predict the future extent of contamination migration from the disposal ponds to the perched water systems and from the perched waste systems to the regional SRPA
 - Design remedial alternatives and evaluate their effectiveness
 - Verify the hydrostratigraphy in which the perched water systems exist.
- The selected model(s) must be verified and reasonably well field tested for conditions similar to those encountered beneath the TRA site
- The selected model(s) must be complete and well documented, should have undergone adequate peer review, and, within reason, should be available in the public domain (proprietary models should be available to public agencies for review, verification and application).

These criteria are based on general criteria established as EPA policies by working groups consisting of nationally-recognized modeling committees (Van der Heijde and Park 1986), and on Site-specific conditions and project objectives.

3.3 Model-Selection Results

This section discusses the model-selection process and results. The section also contains recommendations on the appropriate models for use at TRA.

3.3.1 Groundwater Flow and Contaminant-Transport Models

There are several different types of flow and transport models. Analytical models embody mathematical solutions to the equations that govern groundwater flow and contaminant transport. Numerical models embody approximations to the governing equations using finite-difference or finite-element techniques. Stochastic models contain descriptions of groundwater flow and contaminant transport in terms of statistics and statistical distributions, and they often employ a combination of statistical and numerical methods. Compartmental models incorporate the law of mass conservation, and are composed of a combination of numerical and statistical methods. However, the compartmental models do not solve the groundwater flow and contaminant-transport equations. For

the purposes of modeling flow and transport at the TRA site, analytical, stochastic and compartmental models are considered too simplistic, and are not presented or discussed in this document.

Numerical groundwater flow and contaminant-transport models that are potentially applicable to the site are listed and described in Tables 1 and 2. The information in these tables was obtained from Van der Heijde et al. (1988); Bond and Hwang (1988); Faust et al. (1990) and Dames & Moore (1985). The models in these tables were selected based on general processes that are thought to occur at the TRA: unconfined flow, unsaturated and saturated flow, horizontal and vertical flow, sorption, radioactive flow and density-coupled flow. All of the numerical models (finite difference and finite element) can simulate unconfined flow, contaminant transport, and incorporate adsorption (MODPATH is the only exception: it is a particle-tracking model, and thus, cannot incorporate hydrodynamic dispersion or adsorption).

Table 1 lists important information about each model, and is arranged according to the type of model (finite difference or finite element). Within each type, the models are listed alphabetically according to the name of the model. Table 2 gives a general description of each model. Table 2 is ordered the same as Table 1 (the finite difference models are listed first in alphabetical order), except that the models are listed in groups of five for ease of reading. Table 3 indicates whether each model satisfies the four selection criteria listed in section 3.2.4.

Based on the results of the application of the four criteria (Table 3), three groundwater flow and contaminant-transport models were selected for further evaluation: FLAMINCO, PORFLOW, and TARGET.

FLAMINCO is a three-dimensional, finite-element model, developed by GeoTrans, Inc. The code is well documented and verified. Its history of use is limited. FLAMINCO is a powerful model, and has preprocessing capability but no post-processing capability. FLAMINCO is proprietary (the availability of the code to public agencies is limited). It can handle any condition likely to be encountered at the TRA except for density-coupled flow.

PORFLOW is a three-dimensional finite difference model, developed by ACRI. The code seemed to have been updated quicker than the documentation (Hall et al, 1990) but the code is well verified. It has been used widely PORFLOW is a powerful model with a user-friendly, key word oriented preprocessor. Another ACRI program, ACRPLOT can be used for plotting results. It can handle any conditions likely to be encountered at the TRA.

TARGET is a set of integrated finite-difference models designed to handle a wide variety of modeling situations, and developed by Dames & Moore (1985). The suite of TARGET models all have similar input/output characteristics, and an advanced post-processing capability (for interpretation of results and plotting). The similarity between the models also makes conversion from one model to another (such as converting from two-dimensional to three-dimensional modeling). TARGET is well documented, tested, and verified, and has been used for many DOE and EPA projects. TARGET is available to public agencies, including documentation, executable and source codes, and verification cases under a license agreement for a minor license/support fee. The TARGET models would be applicable to known situations encountered at the TRA.

Table 1. Relevant groundwater flow and transport models for risk assessment.

Name	Source ^a	Spatial dimensionality	Orientation ^b	Type ^c	Public domain code?
BIOPLUME II	RU	2	H	FD	No
HST3D	USGS	3	—	FD	Yes
IDNMIG	SNL	2	H?	FD	No
MOC	USGS	2	H	FD	Yes
MOCNRC	USGS	2	H	FD	Yes
MODFLOW	USGS	3	—	FD	Yes
MODPATH	USGS	3	—	FD	Yes
PORFLOW	ACRI	3	—	FD	No
SATRA-CHEM	USGS	2	H,V?	FD	Yes
SWANFLOW	GEOTRANS	3	—	FD	No
SWIFT	ANL	3	—	FD	No
SWIPR	USGS	3	—	FD	Yes?
TARGET	D&M	1,2,3	H,V	FD	No
TRACR3D	LANL	3	—	FD	No
TRUST	?	1,2,3	—	FD	Yes
FLOTRA	ACRI	2	H,V	FD?	No
FTWORK	GEOTRANS	3	—	FD	Yes
GASOLINE	USGS	1	V	FD?	Yes
MMT-DRPW	PNL	3	—	FD?	No
VADOSE	ACRI	2	H,V	FD?	No
CFEST	PNL	3	—	FE	No
CHAI NT	RI	2	H,V?	FE	No
DSTRAM	HGLI	2,3	H,V	FE	No
FECWASTE	ORNL	2	V	FE	No
FEMTRAN	SNL	2	V	FE	No
FEMWASTE	ORNL	2	H	FE	No
FLAMINCO	GEOTRANS	3	—	FE	No
GGCP	GA	2	H	FE	No?
GREASE2	GEOTRANS	3	—	FE	No
GROWKWA	DHL	2	H	FE	No
GS2	WWLI	2	H,V	FE	No
GS3	WWLI	3	—	FE	No

Table 1. (continued).

Name	Source ^a	Spatial dimensionality	Orientation ^b	Type ^c	Public domain code?
MAQWQ	UA	3?	?	FE	Yes?
MOFAT	EST	2	H,V	FE	No
MOTIF	AEC	1,2,3	—	FE	No
ROCMAS-HS	LBL	2	H?	FE	No
SATURN2	GEOTRANS	2	V	FE	No
SEFTRAN	GEOTRANS	2	H	FE	No
SEGOL	BECHTEL	3	—	FE	Yes
SHALT	INTERA	2	H	FE	No
SOTRAN	UPH	2	H?	FE	No
SUTRA	USGS	2	H,V	FE	Yes
TRAFRAP-WT	IGWMC	2	H	FE	Yes?
TRANQL	LANL	1	H?	FE	No
VAM2D	HGLI	2	H,V	FE	No

a. Source Acronyms:

ACRI - Analytic and Computation Research, Inc.

AEC - Atomic Energy of Canada

ANL - Argonne National Laboratory

BECHTEL - Bechtel Corporation

BMI - Battelle Memorial Institute

D&M - Dames & Moore

DHL - Delft Hydrologic Lab

EPA - U.S. Environmental Protection Agency

EST - Environmental Services and Technology

GA - Golder Associates

GeoTrans - GeoTrans, Inc.

HGLI - HydroGeologic, Inc.

IGWMC - International Ground Water Modeling Center

INTERA - INTERA, Inc.

ISWS - Illinois State Water Survey

LANL - Los Alamos National Laboratory

LBL - Lawrence Berkley Laboratory

ORNL - Oak Ridge National Laboratory

PNL - Pacific Northwest Laboratory

RI - Rockwell International

RU - Rice University

SNL - Sandia National Laboratory

UA - University of Arizona

UPH - University of Port Harcourt

USGS - U.S. Geological Survey

WWLI - Waste, Water and Land, Inc.

b. Orientations:

H - horizontal

V - vertical (cross sectional)

"-" - 3-D model

c. Model Types:

FD - finite difference numerical

FE - finite element, numerical

Note: model types may be mixed.

?: Unsure, but likely.

Table 2. Model capabilities numerical model descriptions.

Name ^a	Decay ^b	Variably saturated	Density coupled	Heat-flow coupled	Multiphase flow	Chemical reactions	Ion exchange	Biodegradation
BIOPLUME II	No	No	No	No	No	No	No	Yes
HST3D	Yes	No	Yes	Yes	No	No	No	No
IDNMIG	Yes (C?)	No	No	No	No	No	No	No
MOC	Yes	No	No	No	No	No	No	No
MODFLOW	No	No	No	No	No	No	No	No
MOCNRC	Yes (C?)	No	No	No	No	No	No	No
MODPATH (*)	No	No	No	No	No	No	No	No
PORFLOW	Yes	Yes	Yes	Yes	Yes	No	No	No
SATRA-CHEM	No	No	No	No	No	Yes	Yes	No
SWANFLOW	No	Yes	No	No	Yes	No	No	No
SWIFT	Yes	No	Yes	Yes	No	Yes	Yes	No
SIWPR	No	No	Yes	Yes	No	No	No	No
TARGET	Yes	Yes	Yes	Yes	No	No	No	No
TRACR3D	Yes	No	No	No	Yes	No	No	No
TRUST	Yes	Yes	No	No	No	No	No	No
FLOTRA	Yes	Yes	Yes	Yes	No	Yes	No	No
FTWORK	Yes	No	No	No	No	Yes	No	No
GASOLINE	Yes	Yes	No	No	Yes	No	No	Yes
MMT-DRPW	Yes	No	No	No	No	Yes	Yes	No

Table 2. (continued).

Name ^a	Decay ^b	Variably saturated	Density coupled	Heat-flow coupled	Multiphase flow	Chemical reactions	Ion exchange	Biodegradation
VADOSE	Yes	Yes	Yes	Yes	No	Yes	No	No
CFEST	Yes	No	Yes	Yes	No	No	No	No
CHAI NT (*)	Yes (C)	No	Yes	No	No	No	No	No
DSTRAM	Yes	No	Yes	Yes	No	No	No	Yes
FEMTRAN (*)	Yes (C)	Yes	No	No	No	No	No	No
FEMWASTE (*)	Yes	No	No	No	No	No	No	Yes
FECWASTE (*)	Yes	No	No	No	No	No	No	Yes
FLAMINCO	Yes	Yes	No	No	No	No	No	No
GGCP	Yes	No	No	No	No	Yes	No	No
GREASE2	No	No	Yes	Yes	No	No	No	No
GROWKWA	Yes	No	No	No	No	Yes	Yes	No
GS2	Yes	Yes	No	No	No	No	No	No
GS3	No	Yes	No	No	No	No	No	No
MAQWQ (*)	Yes	No	No	No	No	No	No	No
MOFAT	Yes	Yes	Yes	No	Yes	No	No	No
MOTIF	Yes	Yes	No	Yes	No	No	No	No
ROCMAS-HS (*)	Yes	No	No	No	No	Yes	No	No
SATURN2	Yes	Yes	No	No	No	Yes	No	No
SEFTRAN	No	No	Yes	Yes	No	No	No	No

Table 2. (continued).

Name ^a	Decay ^b	Variably saturated	Density coupled	Heat-flow coupled	Multiphase flow	Chemical reactions	Ion exchange	Biodegradation
SEGOL	Yes	Yes	No	No	No	No	No	No
SHALT	Yes	Yes	Yes	Yes	No	Yes	No	No
SOTRAN	Yes	No	No	No	No	No	No	Yes
SUTRA	No	Yes	Yes	Yes	No	Yes	No	No
TRAFRAP-WT	Yes	No	No	No	No	Yes	No	No
TRANQL	No	No	No	No	No	Yes	Yes	No
VAM2D	Yes	Yes	No	No	No	No	No	Yes

a. "*" indicates a model that requires the output from another model.

b. "C" indicates a model that incorporates chain decay.

Table 3. Models versus selection criteria.

Name	Satisfaction of selection criteria ^a			
	1	2	3	4
BIOPLUME II	Y	N	N	Y
HST3D	N	Y	Y	Y
IDNMIG	Y	Y	N	N
MOC	N	N	Y	Y
MOCNRC	N	N	Y	Y
MODFLOW	N	N	Y	Y
MODPATH	Y	N	Y	Y
PORFLOW ^b	Y	Y	Y	Y
SATRA-CHEM	Y	N	N	Y
SWANFLOW	Y	N	Y	Y
SWIFT	N	Y	Y	Y
SWIPR	N	N	N	N
TARGET ^b	Y	Y	Y	Y
TRACTR3D	N	N	N	N
TRUST	Y	Y	Y	N
FLOTRA	Y	Y	N	N
FTWORK	N	Y	Y	Y
GASOLINE	N	N	N	Y
MMT-DRPW	Y	Y	N	N
VADOSE	Y	Y	N	N
CFEST	N	Y	Y	Y
CHAI NT	Y	N	N	N
DSTRAM	Y	Y	N	N
FECWASTE	Y	Y	N	Y
FEMTRAN	Y	Y	N	N
FEMWASTE	Y	Y	N	Y
FLAMINCO ^b	Y	Y	Y	Y

Table 3. (continued).

Name	Satisfaction of selection criteria ^a			
	1	2	3	4
GGCP	N	N	Y	Y
GREASE2	N	N	Y	Y
GROWKWA	Y	Y	N	N
GS2	Y	Y	N	N
GS3	N	N	N	N
MAQWQ	N	N	N	N
MOFAT	Y	N	Y	Y
MOTIF	Y	N	Y	N
ROCMAS-HS	Y	Y	N	N
SATURN2	Y	Y	N	N
SEFTRAN	N	N	Y	N
SEGOL	Y	Y	Y	N
SHALT	Y	Y	Y	N
SOTRAN	Y	Y	N	N
SUTRA	Y	N	Y	Y
TRAFRAP-WT	Y	Y	N	Y
TRANQL	N	N	N	N
VAM2D	N	Y	Y	Y

a. Selection criteria (Section 4.2.4):

1. Model is capable of simulating site transport and flow conditions.
2. Model is capable of accomplishing study objectives.
3. Model has been verified and field tested.
4. Model has been adequately reviewed, is well documented, and is available.

b. Satisfies all four criteria.

On the basis of the above discussion of the models, the TARGET models were selected to model the TRA. The main reasons were

- TARGET has a comprehensive suite of post-processing programs designed to aid in the display and interpretation of results
- A direct conversion can be made from the initial two-dimensional cross-sectional model to the three-dimensional model
- It is readily available with complete documentation and validation cases
- TARGET has been applied to over 120 projects
- TARGET is the most comprehensive and complete of the three models, capable of modeling unsaturated, density-coupled, flow, transient flow and transport and variable contaminant sources, and sinks.

4. DATA REQUIREMENTS FOR MODELING

Flow and transport models require hydrogeologic, water-quality, and meteorologic data. For the TRA Perched Water System, the specific data requirements for groundwater flow and contaminant-transport models are listed below.

Fluids and Contaminants

- Background or initial concentrations of dissolved/suspended species
- Spatial and temporal measurements of concentrations
- Types of dissolved/suspended species
- Decay constants for radioactive and organic species
- Molecular diffusion coefficients
- Fluid density and viscosity as a function of concentration
- Geochemical data (solubility, concentrations of major and minor ions, potential reactions or nature of mixing liquids, Henry's constant, etc.).

Hydrogeologic Conditions

- Distribution of hydrostratigraphic units
- Saturated thickness
- Unsaturated thickness
- Hydraulic conductivities (for all materials if necessary and for saturated and unsaturated conditions), including the distribution and hydraulic characteristics of fractures
- Anisotropy of hydraulic conductivity
- Moisture characteristic curves (unsaturated zone)
- Nature and distribution of clays (for both transport and geochemical models)
- Organic carbon content
- Effective porosity (primary and fracture)
- Dispersivities
- Specific storage coefficients (primary and fracture)

- Nature and distribution of important minerals (if any)
- Adsorption distribution coefficients (K_d)
- Ion exchange capacities
- Soil/rock bulk densities
- Retardation factors (a function of K_d , porosity, and bulk density)
- Topographic information
- Meteorologic data (precipitation rates, temperature, humidity, etc.)
- Locations of hydraulic head and concentration measurements
- Measurements of hydraulic head (spatial and temporal)
- Distribution, duration, and rates of natural and artificial recharge (boundary conditions)
- Distribution, duration, and rates of natural and artificial discharge (boundary conditions)
- Distribution, duration, rates, concentration, and constituents of contaminant sources (boundary conditions).

Model

- Domain size (location of sources and receptors)
- Spatial grid or mesh
- Time increment
- Simulation period.

Based on the review of the available information, all of the above listed information is or will be available from field activities or from published sources. In general, model predictions are most sensitive to framework/material properties, boundary conditions, and contaminant sources/sinks; thus, these data are the most important.

4.1 Results of Evaluation

The model data requirements for each model are listed in Figure 5. Results of the data evaluation are discussed in the following paragraphs and are listed in Table 4. In general, most required data for groundwater and contaminant-transport modeling have been or will be measured

	FRAMEWORK MATERIAL PROPERTIES	BOUNDARY CONDITIONS (RECHARGE/DISCHARGE)	SINKS	HYDRAULIC HEAD SATURATED THICKNESS	CONCENTRATIONS	ADSORPTION	DECAY/DEGRADATION	GEOCHEMISTRY	UNSATURATED ZONE PARAMETERS	MULTI-PHASE FLOW PARAMETERS
BIOPUME II	•	•	•	•	•	•				
HST3D	•	•	•	•	•	•				
IDNMIG	•	•	•	•	•	•				
MOC	•	•	•	•	•	•				
MOCNRC	•	•	•	•	•	•				
MODPATH	•	•	•	•	•	•				
SATRA-CHEM	•	•	•	•	•	•	•			
SWANFLOW	•	•	•	•	•	•		•		
SWIFT	•	•	•	•	•	•				
SWIPR	•	•	•	•	•	•				
TARGET	•	•	•	•	•	•		•		
TRACR3D	•	•	•	•	•	•			•	
TRUST	•	•	•	•	•	•		•		
FLOTRA	•	•	•	•	•	•		•		
FTWORK	•	•	•	•	•	•		•		
GASOLINE	•	•	•	•	•	•		•		
MMT-DRPW	•	•	•	•	•	•		•		
VADOSE	•	•	•	•	•	•		•		
CFEST	•	•	•	•	•	•				
CHAIT	•	•	•	•	•	•				
DSTRAM	•	•	•	•	•	•				
FECWASTE	•	•	•	•	•	•				
FEMTRAN	•	•	•	•	•	•		•		
FEMWASTE	•	•	•	•	•	•				
FLAMINCO	•	•	•	•	•	•		•		
GGCP	•	•	•	•	•	•		•		
GREASE2	•	•	•	•	•	•				
GROWKWA	•	•	•	•	•	•		•		
GS2	•	•	•	•	•	•		•		
GS3	•	•	•	•	•	•		•		
MAQWQ	•	•	•	•	•	•				
MOFAT	•	•	•	•	•	•		•		
MOTIF	•	•	•	•	•	•		•		
PORFLOW	•	•	•	•	•	•		•		
ROCMAS-HS	•	•	•	•	•	•		•		
SATURN2	•	•	•	•	•	•		•		
SEFTRAN	•	•	•	•	•	•				
SEGOL	•	•	•	•	•	•		•		
SHALT	•	•	•	•	•	•		•		
SOTRAN	•	•	•	•	•	•				
SUTRA	•	•	•	•	•	•		•		
TRAFRAP-WT	•	•	•	•	•	•		•		
TRANQL	•	•	•	•	•	•		•		
VAM2D	•	•	•	•	•	•		•		

• - Data Required

Figure 5. Data requirements for the groundwater flow and transport models.

Table 4. Data requirements versus data availability.

Data type	Needed ^a	Site wide ^b	Local ^c	Sparse ^d	Literature/ unknown ^e
Fluids and contaminants					
Background/initial concentrations	•	•	•	•	—
Temporal concentrations	•	•	•	—	—
Types of species	•	•	•	•	—
Decay constants	•	—	—	—	•
Molecular diffusion coefficients	•	—	—	—	•
Density/viscosity of fluids	•	•	•	—	•
Geochemical data	•	•	•	•	•
Hydrogeologic conditions					
Distribution of hydrostratigraphic units	•	•	•	—	—
Saturated thickness	•	•	•	—	—
Unsaturated thickness	•	•	•	—	—
Hydraulic conductivities/fracture characteristics	•	•	•	• ^f	• ^g
Anisotropy	•	—	•	—	•
Moisture-characteristic curves	•	•	•	—	—
Nature and distribution of clays	•	•	•	•	•
Organic carbon content	•	•	•	—	• ^h
Effective porosity	•	•	•	• ^f	• ^g
Dispersivities	•	•	•	•	•
Specific storage coefficients	•	•	•	• ^f	• ^g
Nature and distribution of important minerals	•	•	•	•	•
Adsorption distribution coefficients	•	•	—	—	•
Ion exchange capacities	•	•	•	—	—
Bulk densities	•	•	•	—	—
Retardation factors ⁱ	•	—	—	—	—
Topography	•	—	•	—	—
Meteorological data	•	•	—	—	•
Water levels ^j	•	•	•	—	—

Table 4. (continued).

Data type	Needed ^a	Site wide ^b	Local ^c	Sparse ^d	Literature/ unknown ^e
Natural/artificial recharge	•	•	•	—	—
Natural/artificial discharge	•	•	•	—	—
Characteristics of contaminant sources	•	•	•	—	—
Model^k					
Domain size	•	—	•	—	—
Spatial grid	•	—	•	—	—
Time increment	•	—	•	—	—
Simulation period	•	—	•	—	—

a. Is the data required to model the TRA site?

b. Site Wide: Data available from other INEL sites or investigations.

c. Local: Data are available for the TRA site.

d. Sparse: Only a limited amount of data is available for the TRA site. There are categories in which more data may be required.

e. Literature/unknown: No data are available. In some cases, published data can be substituted.

f. No specific requirements have been identified with respect to characterizing the hydraulic properties of fractures and other secondary processes.

g. The hydraulic properties of fractures may be assessed and estimated based on published data.

h. Organic carbon content will be used to assess the ability of organic matter to absorb organic and other contaminants.

i. Retardation factors can be calculated from other data.

j. Spatial and temporal measurements of hydraulic head.

k. Specific model setup is based on site-specific data and interpretations of it.

both locally and site-wide. The existing data set combined with ongoing and planned data-collection activities are adequate to meet the needs of groundwater flow and contaminant-transport modeling (providing that the data meet the data-validation requirements of the project). The use of historic data (data collected before the current characterization program, namely by the USGS) has been limited because of the lack of information supporting the quality of those results. However, these data used in conjunction with the 1991 data set will provide a means of detecting and estimating trends and contaminant-specific transport characteristics. The 1991 chemical data set provides a comprehensive suite of potential contaminants and concentrations. These data will be used to select the subset of constituents to be modeled.

At this time, there are enough data to evaluate the nature and distribution of contaminants in the subsurface. A complete set of geochemical data are being collected for the deep perched water zone and the SRPA. No further data requirements in this area have been identified.

Existing data will be used to characterize the subsurface geochemical environment and the Site conditions and processes that affect the movement of contaminants through the geologic environment. At this time, no further data collection activities in this area are recommended.

Existing data will be used to qualitatively characterize the fracture system in the basalt beneath the Site. To assess the importance of fracturing, sensitivity analyses will be performed using the contaminant-transport model and data from other sites at the INEL. As the data are more completely analyzed, further data needs in this area may be identified; however, currently there are no plans to collect additional information.

Barometric pressure measurements should be made coincident with the water-level measurements. Such information can be used to characterize the storage coefficient and specific yield of saturated units. The collection of this data is currently underway.

The 1991 sampling and analysis program was designed to characterize the nature and distribution of clays, important minerals, and solid organic matter. The program was also designed to characterize the effective porosity, specific yield, storage coefficient, vertical and horizontal hydraulic conductivity of the key hydrogeologic units, and vertical and horizontal hydraulic gradients. This information will be used for the Perched Water System RI/FS.

Adsorption of contaminants by subsurface clays and oxyhydroxide minerals is important because large quantities of contaminants can be adsorbed, adsorption properties are highly Site-specific, and desorption can play an important role during the cleanup of contaminants. There are no current plans to collect Site-specific information on the adsorption properties of these solids. Adsorption distribution coefficients will be obtained from published information from geohydrologically similar sites. A sensitivity analysis can be conducted, during the modeling activity, to assess the impact of adsorption and desorption on the transport of contaminants. It is expected that adsorption will have a small impact on the overall model predictions because of the low concentration of contaminants in the deep perched water zone and the SRPA and the adsorption coefficients are high for the contaminants that have been identified.

The geochemical characteristics of the pond sediments will be required to understand the rates of and mechanisms affecting contaminant migration from the ponds into the subsurface. The

necessary information may be provided by ongoing or planned feasibility study activities for the ponds at TRA. At this time, no further data needs in this area have been identified.

With respect to the most important data, namely, framework/material properties, boundary conditions, and contaminant sources/sinks, there is enough data to proceed with the Perched Water System RI/FS modeling activities. No further data requirements have been identified at this time. This conclusion is based on an evaluation of the existing information and ongoing and planned data-collection activities, and it is based on the assumption that the data will meet the requirements of the project data validation criteria.

5. SUMMARY AND CONCLUSIONS

In order to model these hydrogeologic conditions and the contamination characteristics at TRA, several groundwater flow and contaminant-transport models have been evaluated for their applicability. Model selection was based on four criteria

1. The selected model(s) must be able to adequately simulate site conditions
2. The selected model(s) must be able to satisfy the objectives of the study
3. The selected model(s) must be verified, and reasonably well field tested
4. The selected model(s) must be well documented, peer reviewed and available.

Based on these criteria and detailed model evaluations, the TARGET model is recommended for TRA. The TARGET_2DU can be used for the initial investigation and TARGET_3DU can be used for detailed Site modeling. Both the models require similar types of input; therefore, it is an easy task to incorporate the results of the TARGET_2DU model into the more complicated TARGET_3DU model.

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Appendix A

Brief Description of Mathematical Background of the TARGET Models

Appendix A

Brief Description of Mathematical Background of the TARGET Models

INTRODUCTION

This appendix summarizes the groundwater flow and solute transport mechanisms, mathematical formulation, and mathematical framework of a numerical model. The model simulates groundwater flow and chemical-species transport in variably saturated porous media. The mathematical model described, developed by Dames & Moore over the past eight years, is known as TARGET (Transient Analyzer of Reacting Groundwater and Effluent Transport). This document provides a general description of the methodology and assumptions employed in the model, and places the mathematical technique in context with a brief outline of current literature on the subject.

Documents covering details of the mathematical formulation, model input data structure and definitions, and validation cases covering the range of model applicability are available separately (Dames & Moore 1985a and b). This appendix relates to three of the five models in the TARGET family: TARGET_2DU (two-dimensional, vertical cross section, variably saturated), TARGET_3DU (three-dimensional, variably saturated), and TARGET_3DS (three-dimensional, fully saturated). These programs, together with the mathematical formulation and numerical technique, are collectively referred to as the model (or TARGET) in the following pages.

The technology of mathematical models that predict fluid flow and solute transport has advanced rapidly in recent years. The number of variably-saturated flow and solute transport models described in published reports increased from two (3D) and four (2D) in 1980 (Lappala 1980) to three (3D) and eleven (2D) in 1985 (Van der Heijde et al. 1985). More than 100 numerical mass transport models were available in 1985 (Van der Heijde et al. 1985). The literature describing these advances has been reviewed and summarized by several authors, including Narasimhan and Witherspoon (1977), Lappala (1980), and Van der Heijde et al. (1985). The numerical techniques employed in these mathematical models include finite element methods (Remson et al. 1971, Pinder and Gray 1977), finite difference methods (Freeze and Cherry 1979), and integrated finite difference methods (Narasimhan and Witherspoon 1976).

Along with the more complex mathematical models comes the need for more detailed site-specific material property information for the adequate representation of the phenomena simulated. Typically, unsaturated material properties are required for flow calculations, and dispersion coefficients and adsorption isotherms are required for transport calculations. Unsaturated material properties are reported for sands (Reisenauer 1963, Vauclin et al. 1975), loams (Reicosky 1981, Safai and Pinder 1979), stony soils (Bouwer and Rice 1984), and a wide range of other soil types (Bouwer 1964, Mualem 1976). Dispersion coefficients, incorporating both molecular diffusion and mechanical dispersion, are usually supplied to models as constitutive relationships involving various physical and numerical assumptions (Sposito et al. 1986). Dispersion coefficients (or dispersivities) may be measured in the laboratory (Klotz and Moser 1974), in the field (Schwartz 1977, Molz et al. 1983),

or inferred from modeling analysis (Anderson 1977, Mercer and Faust 1981). The derivation and use of adsorption isotherms have received considerable attention because of the importance of sorption effects on contaminant distributions and because of the uncertainties involved in commonly-used assumptions. Adsorption theory, in the context of model representation, is discussed in Corey (1981) and Reardon (1981). Contaminant mobilities are described in journals covering several disciplines for radionuclides (Seitz et al. 1978, Battelle Pacific Northwest Laboratories 1978), pesticides (Davidson et al. 1978), organics (Wilson et al. 1981, Chiou et al. 1979), and metals (Huang et al. 1977, Theis et al. 1981).

The mathematical model that is developed should be at least as sophisticated as the level of the site-specific data available. The mathematical model described herein combines the following with a computationally-economic solution algorithm: (a) the saturated flow capabilities similar to the U.S. Geological Survey (USGS) MODFLOW model (McDonald and Harbaugh 1984), (b) the unsaturated flow capabilities of Lawrence Berkeley Laboratory's TRUST model (Narasimhan 1975), (c) the solute transport capabilities of the USGS SUTRA model (Voss 1984).

The TARGET model capabilities permit application of the model to widely varying conditions. For example, as part of water management and waste disposal projects, the model is routinely applied to

- Provide assistance in siting facilities
- Help in designing facilities (e.g., well fields for water supply; infiltration basins for artificial recharge; landfills for solid waste; impoundments for slurry, tailings, or chemical wastes; or deep burial sites for radioactive wastes)
- Evaluate performance of facilities by predicting the nature of the flow field and the extent and gravity of contaminant migration
- Develop a valid conceptual model of site conditions based on field observations, literature data, and hydrogeologic hypotheses
- Assist in devising effective field measurement and monitoring programs
- Design cleanup and pollution abatement measures for contaminated groundwater and soils
- Demonstrate compliance with regulatory requirements
- Assist in developing closure plans for facilities
- Predict the long-term behavior of waste-disposal facilities.

Models of the TARGET family have been applied in more than 80 projects to a range of water management and contaminant control problems including

- Dewatering multiple aquifers during operation of an Australian strip mine

- Simulating alternate remedial measures at five Superfund sites
- Predicting containment and extracting light hydrocarbons and dense mine wastes.

During the course of these applications, the model approach and predictions have been reviewed and approved by many regulatory agencies including USGS and the U.S. Environmental Protection Agency. In addition, a satisfactory peer review of the model formulation, solicited by Dames & Moore, was given by Professor Allan Freeze (see Appendix B). These review opinions, as well as publications and model validation cases, provide the basis for background substantiation of model predictions.

GROUNDWATER FLOW AND SOLUTE TRANSPORT MECHANISMS

Groundwater Flow

The flow mechanisms simulated by TARGET are

- Unsaturated pore-pressure gradients. For example, the gradients that result in flow between a leaking evaporation pond and the water table.
- Saturated pressure-head gradients. The gradient developed adjacent to a drain is an example of this mechanism.
- Gravity-induced and density-induced gradients. For example, heavy oil may migrate along the base of the aquifer or at an angle to the direction of regional groundwater flow caused by density-induced pressure gradients.
- Aquifer storage changes. For instance, withdrawal of water from a pumping well will result in changes in storage because of depressurization (water will be released from storage because of the compressibility of water and the elasticity of soil matrix) and, if unconfined, dewatering (drainage from the soil pores).

Flow through the unsaturated zone is governed by the unsaturated soil hydraulic characteristics as well as the local pressure gradients. Two parameters are used to define the unsaturated soil characteristics in this model: (a) degree of saturation (S_r), and (b) hydraulic conductivity relative to the saturated hydraulic conductivity (K_r). Both S_r and K_r are a function of pressure head (Figure A-1) and vary with soil type (Figure A-2).

Solute Transport

The transport mechanisms incorporated in TARGET are

- Advection—movement as a result of hydraulic pressure gradients.
- Mechanical dispersion—mechanical mixing or spreading from the tortuosity of flow paths through the soil or rock.
- Molecular diffusion—mixing on a molecular scale because of concentration gradients. Molecular diffusion is a significant component of transport only at low groundwater flow velocities.

Microscopic measurements are not practical on a field scale so an empirical relationship is used in TARGET (and other models) to describe mechanical dispersion and molecular diffusion. The present model uses a widely accepted dispersion relationship described by Huyakorn and Pinder (1982).

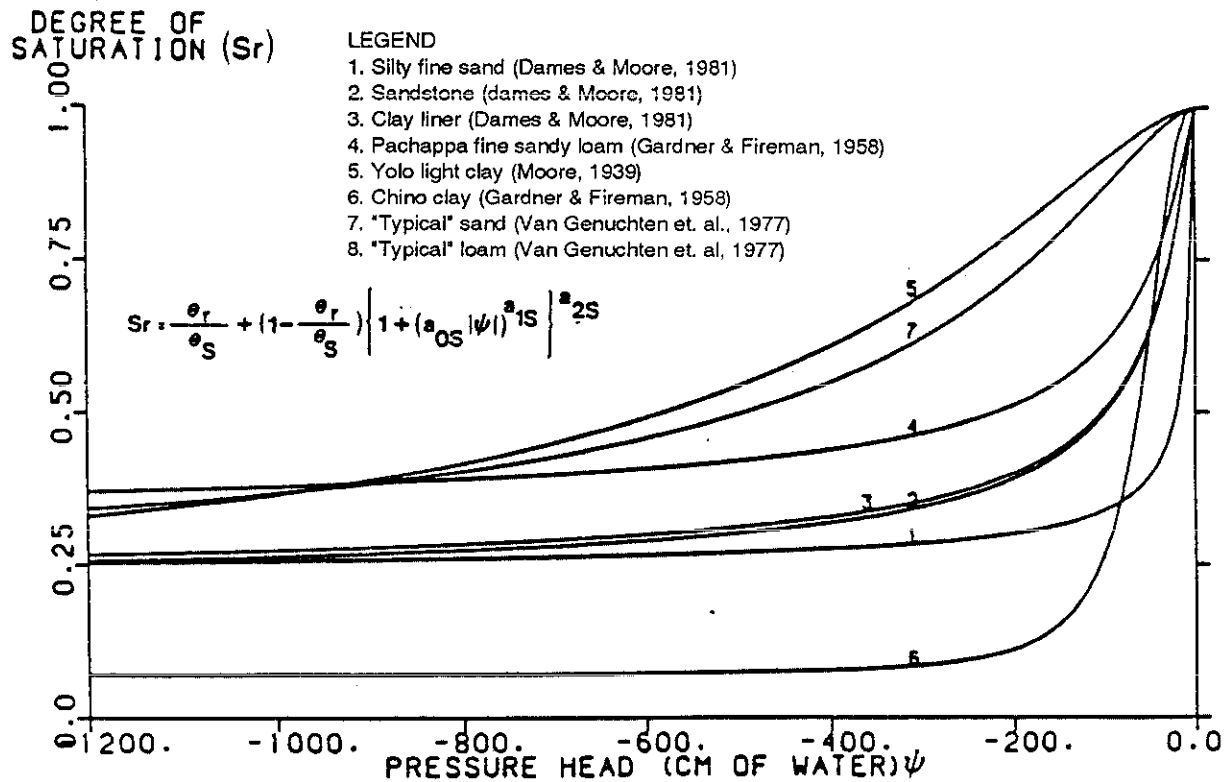
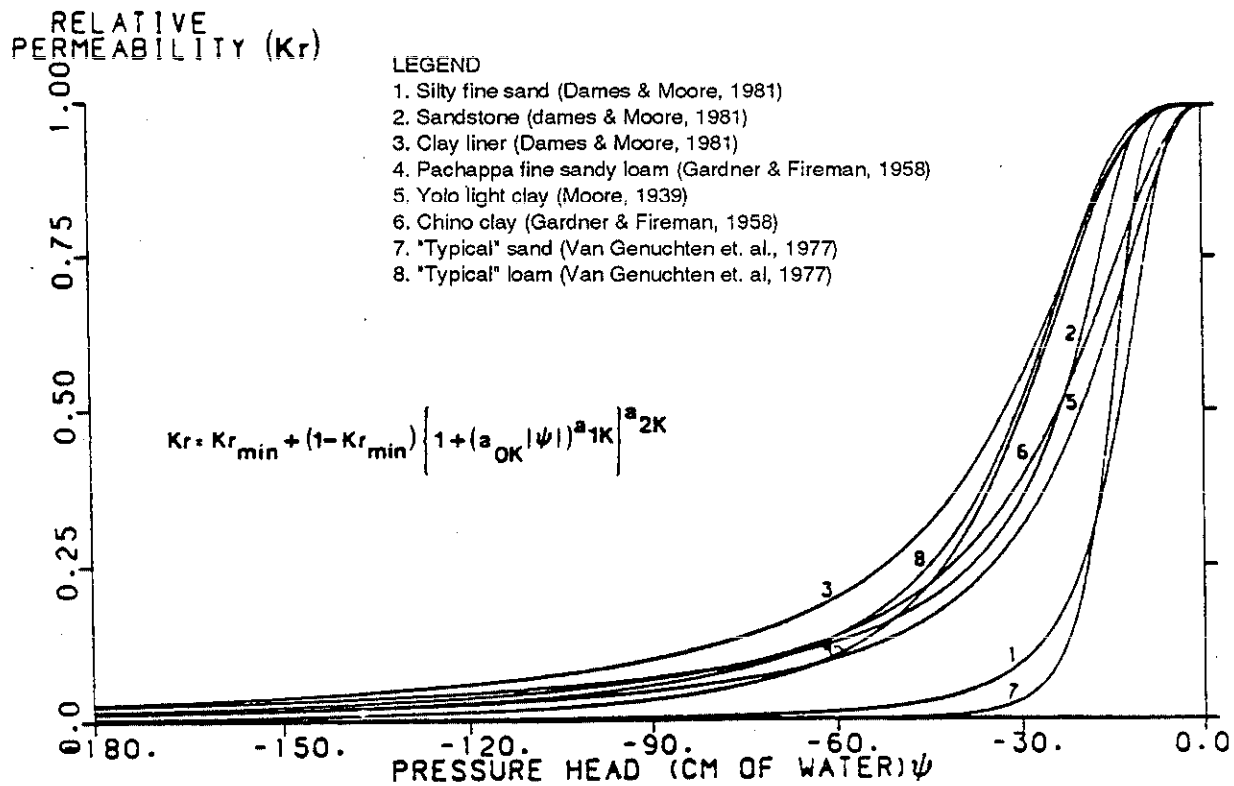


Figure A-1. Relationship for various soils between relative permeability and pressure head, and degree of saturation and pressure head, respectively.

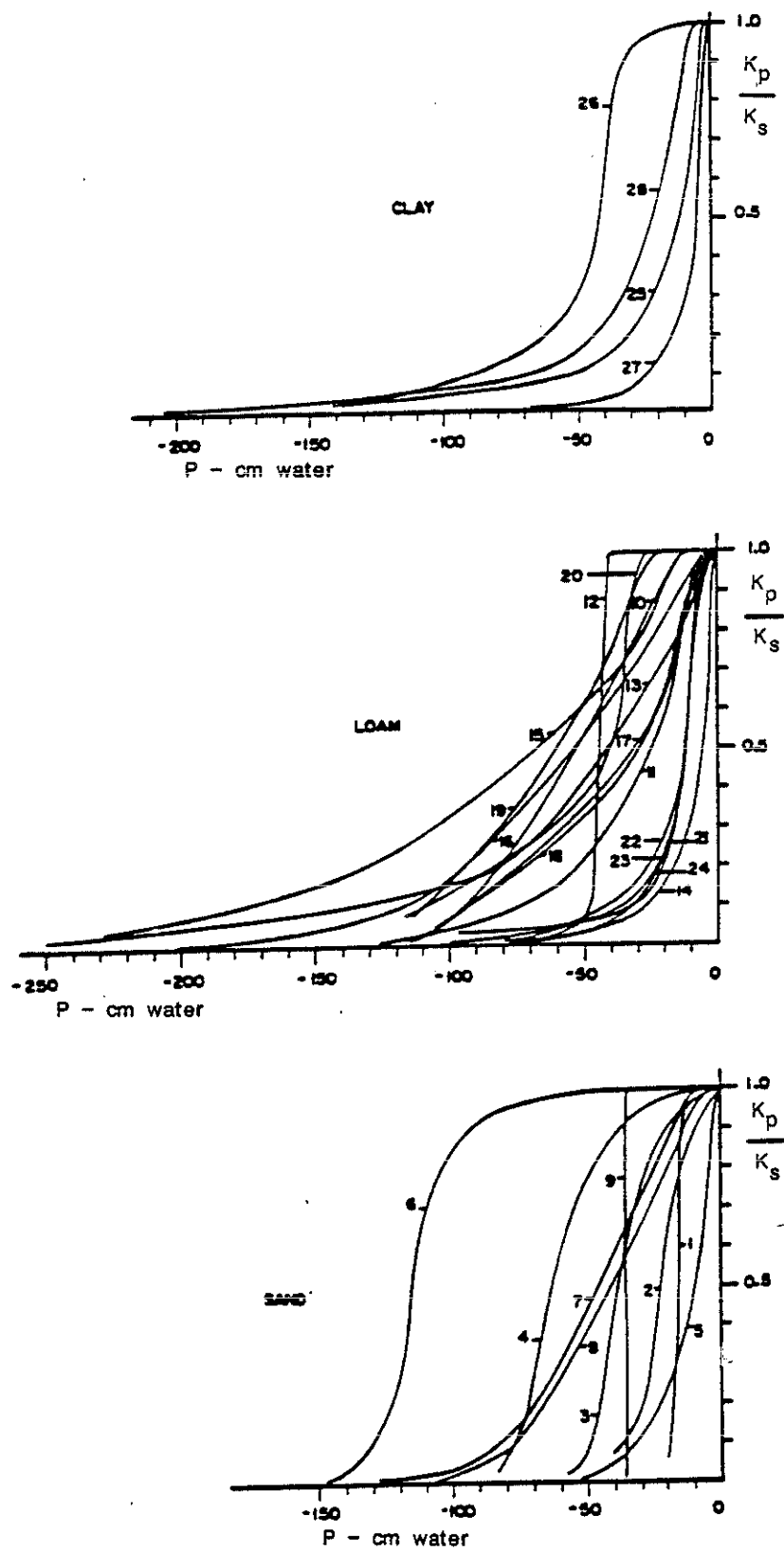


Figure A-2. Unsaturated hydraulic conductivity curves for various soil types.

- Sorption—the immobilization (adsorption) or mobilization (desorption) of solutes through interaction between the soil or rock and the solution in the pores. Such interactions may consist of one or more of the following mechanisms: mechanical filtration, cation exchange, pH buffering, chemical precipitation, hydrolysis, and oxidation-reduction reactions. In characterizing the sorption of solutes, it is important to evaluate the geochemical environment in relation to the solute(s) of interest.

The net effect of these adsorption and desorption interactions is often represented by an equilibrium sorption model, such as the linear adsorption isotherm (Helfferich 1962). The linear adsorption isotherm is used in TARGET, although alternate adsorption isotherms may be incorporated, if appropriate, for a given situation. Evidence suggests that linear adsorption isotherms are representative of organic contaminant behavior for concentrations up to their aqueous solubility (Chiou et al. 1979), but that adsorption of metal contaminants may be strongly dependent on the local pH (Dames & Moore 1981).

- Density effects—density stratification such as might occur in the leakage of light solvents or movement of dense total dissolved solid plumes. Migration of separate-phase liquids (such as gasoline in groundwater) will only be approximately represented by TARGET. Density differences of about 1% are known to significantly influence subsurface fluid movement (Mackay et al. 1985). In the present model, it is assumed that density is proportional to the predicted solute concentration. This assumption is appropriate for organic solutions (Perry and Chilton 1973), as well as for metals and total dissolved solids (Dames & Moore 1983a).

MATHEMATICAL FORMULATION

Governing Equations

Three basic equations govern groundwater flow and solute transport in variably-saturated soils. These are

- Conservation of groundwater flow (i.e., mass conservation of groundwater)
- Darcy's law
- Conservation of chemical product in solution in groundwater (solute), also referred to as the equation of mass transport.

Conservation of Groundwater Flow

The fundamental three-dimensional mass conservation equation for variably-saturated porous media is expressed as follows (Bear 1979):

$$\underbrace{\frac{\partial}{\partial t}(nSr\rho)}_{\text{groundwater storage}} + \underbrace{\frac{\partial}{\partial x_i}(nSr\rho U_i)}_{\text{inflows and outflows}} = \underbrace{\dot{m}'''}_{\text{sources and sinks}} \quad (\text{A-1})$$

where

t = time (T)

n = porosity (-)

Sr = degree of saturation (-)

ρ = density (M/L³)

x_i = i-direction coordinate (L)

U_i = i-direction particle velocity (L/T)

\dot{m}''' = source or sink per unit volume per unit time (M/TL³).

Darcy's Law

The generalized form of Darcy's law in anisotropic porous media can be expressed as follows (Bear 1979)

$$\underbrace{nSrU_i}_{\text{Darcy velocity}} = \underbrace{-Kr \frac{K_{ij}\rho g}{\mu}}_{\text{hydraulic conductivity}} \underbrace{\left(\underbrace{\frac{\partial \psi}{\partial x_j}}_{\text{pressure head gradient}} + \underbrace{\frac{\partial Z}{\partial x_j}}_{\text{elevation head gradient}} \right)}_{\text{total head gradient}} \quad (\text{A-3})$$

where

- K_r = relative conductivity (-)
- k_{ij} = intrinsic conductivity tensor component (L^2)
- g = gravitational acceleration (L/T^2)
- μ = viscosity (M/LT)
- ψ = pressure head (L)
- x_j = j-direction coordinate (L)
- Z = vertical axis (L).

Solute Mass Conservation

The fundamental three-dimensional conservation equation for solute mass concentration in groundwater is expressed as (Bear 1979)

$$\underbrace{\frac{\partial}{\partial t}(nSr\rho m_J)}_{\text{storage in mobile phase}} + \underbrace{\frac{\partial}{\partial t}[(1-n)\rho_s m_{J,s}]}_{\text{storage in immobile phase}} + \underbrace{\frac{\partial}{\partial x_i}(nSr\rho U_i m_J)}_{\text{advection}} = \underbrace{\frac{\partial}{\partial x_i}\left(nSr\rho D_{ij}\frac{\partial m_J}{\partial x_j}\right)}_{\text{dispersion}} + \underbrace{\dot{m}''' M_J}_{\text{sources and sinks}} \quad (\text{A-3})$$

where

- m_J = mass concentration of solute J in groundwater (M/M)

ρ_s = soil bulk density (M/L^3)

$M_{J,s}$ = mass concentration of solute J in soil (M/M)

D_{ij} = dispersion coefficient tensor (L^2/T)

M_J = source mass concentration of solute J (M/M).

Using these three fundamental equations and introducing the concepts of specific storage, equilibrium sorption, and dispersivity, two equations are derived to describe the variation of pressure head (ψ) and mass concentration (m_J) with time (Dames & Moore 1985a).

Guess and Correct Algorithm

The TARGET program uses a "guess and correct" (predictor/corrector) algorithm to solve the pressure head and solute mass concentration equations. In this method, it is assumed that the pressure head variable, for instance, consists of a "guessed" value and a correction to that value. The "guessed" values are either the previous solution or the initial conditions, and the corrections are the unknowns to be solved. This technique is advantageous because the correction is a small number relative to the mean value of pressure or concentration. Therefore, small but highly significant gradients can be accurately simulated even if the mean values are large.

Initial Conditions

Initial conditions for pressure head (ψ) and solute mass concentration (m_J) are required either as (a) an initial estimate of the solution to a steady-state calculation or (b) existing conditions for the startup of transient predictions.

The initial conditions can be derived from observed or postulated field conditions or by calculating a steady-state or transient distribution (assuming appropriate boundary conditions). It is important to establish well-balanced initial conditions before calculating transient or time-dependent variations. If good initial conditions are not provided, the transient calculations may result in unwanted pressure or solute mass redistribution at early times. In most cases, a preliminary steady-state or transient calculation is performed to provide the initial conditions for a predictive calculation.

Boundary Conditions

Boundary conditions for pressure head and solute mass concentration are required to complete the definition of the site conditions. The various types of boundary conditions encountered in flow and solute transport through soil and rock are

- Prescribed boundary values. The pressure head or solute concentrations are assigned a prescribed value along the entire boundary or sections thereof. This type of boundary condition is also called a Dirichlet boundary condition.

- Prescribed boundary flux. On a boundary of this type, the flux (flow rate) of groundwater or solute perpendicular to the boundary is prescribed. A special case of this type of boundary is the impervious boundary where the flux is zero. This type of boundary condition is also called a Neumann boundary condition.

Other types of boundary conditions, such as Cauchy (also called mixed boundary conditions), can be represented by combinations of the above two types. All of the boundary condition values may vary with time.

Internal Sources and Sinks

Practical problems often require the representation of man-made or natural features such as wells, rivers, lakes, ponds, infiltration, or evaporation. This is generally achieved by using internal sink or source terms, or by using prescribed values within the calculation domain (as opposed to prescribed values on the boundary of the calculation domain). Sources and sinks may vary with time.

NUMERICAL METHODS

An integrated finite-difference (IFD) calculation procedure is used to solve the equation set. A grid system consisting of rectangular cells of arbitrary length-to-width ratio, with grid nodes located at the geometrical center of each cell, serves as the basis for the derivation of the discretized (i.e., IFD) equations. The finite difference equations are obtained by integrating the fundamental differential equations over each of the cells in the calculation domain. This procedure transforms the partial differential equations into two sets of algebraic linearized equations: one for the calculation of pressure head, and the other for the calculation of mass concentrations.

When integrating the mass transport equation, careless use of central differencing techniques can lead to unstable or physically meaningless solutions when the problem is advection-dominated (Peclet number greater than one^a). In the present model, such difficulties are overcome with a hybrid differencing scheme in which backward, forward, or central differencing schemes are used, depending on the local Peclet number and direction of flow.

When integrating the flow equation, evaluation of the degree of saturation also requires care because (a) it is a strongly nonlinear coefficient sensitive to changes in pressure head and (b) it is closely linked to the relative hydraulic conductivity. Since the degree of saturation versus pressure head relationship is strongly nonlinear, it would be inaccurate to calculate the average degree of saturation of a calculation cell solely on the basis of the predicted pressure head at the node. To minimize such inaccuracy, it is common practice to use a large number of small calculation cells in the unsaturated zone. In the present model, the average degree of saturation is calculated on the basis of an assumed linear variation of pressure head between nodes along the vertical axis.

a. Peclet number is defined here as the magnitude of the ratio of the advective term over the diffusive term.

SOLUTION TECHNIQUES

Iterative Method

Since the pressure head equation is nonlinear, and since density and viscosity effects may create strong coupling between the pressure head and the mass concentration equations, an iterative solution method is required.

The iteration scheme used in TARGET is composed of three levels of iteration. These levels, discussed below, are also illustrated in Figure A-3:

1. The main iteration loop, over the solution of both the pressure head and mass concentration equations. The objective of this loop is to account for the density and viscosity coupling effects.
2. The secondary iteration loop over the solution of the equations of pressure head and mass concentration individually. The objective of this loop is to account for the nonlinear terms such as relative conductivity and degree of saturation.
3. The innermost iteration loop is the matrix solution loop. The objective of this loop is to obtain an accurate solution for a given set of coefficients.

The convergence of these various loops is tested to establish when an accurate solution is obtained.

Matrix Solution Algorithm

The solution algorithm implemented in TARGET is based on an alternating direction implicit (ADI) algorithm. In two-dimensional problems, the ADI is implemented as a line-by-line, column-by-column solution sequence of the resulting three-diagonal matrix. In three-dimensional problems, the same alternating direction scheme is used, but all planes are solved simultaneously, which results in the solution of a five-diagonal matrix.

Each solution sweep is composed of the following steps:

- Assemble the three-dimensional matrix with a suitable combination of terms
- Apply a forward elimination, backward substitution algorithm to the resulting matrix
- Repeat sequence an even number of times to achieve a complete solution.

Relaxation

In the guess and correct formulation described, the dependent variable is a correction that must be added to the previous solution of the primary variable. A fully converged solution is obtained

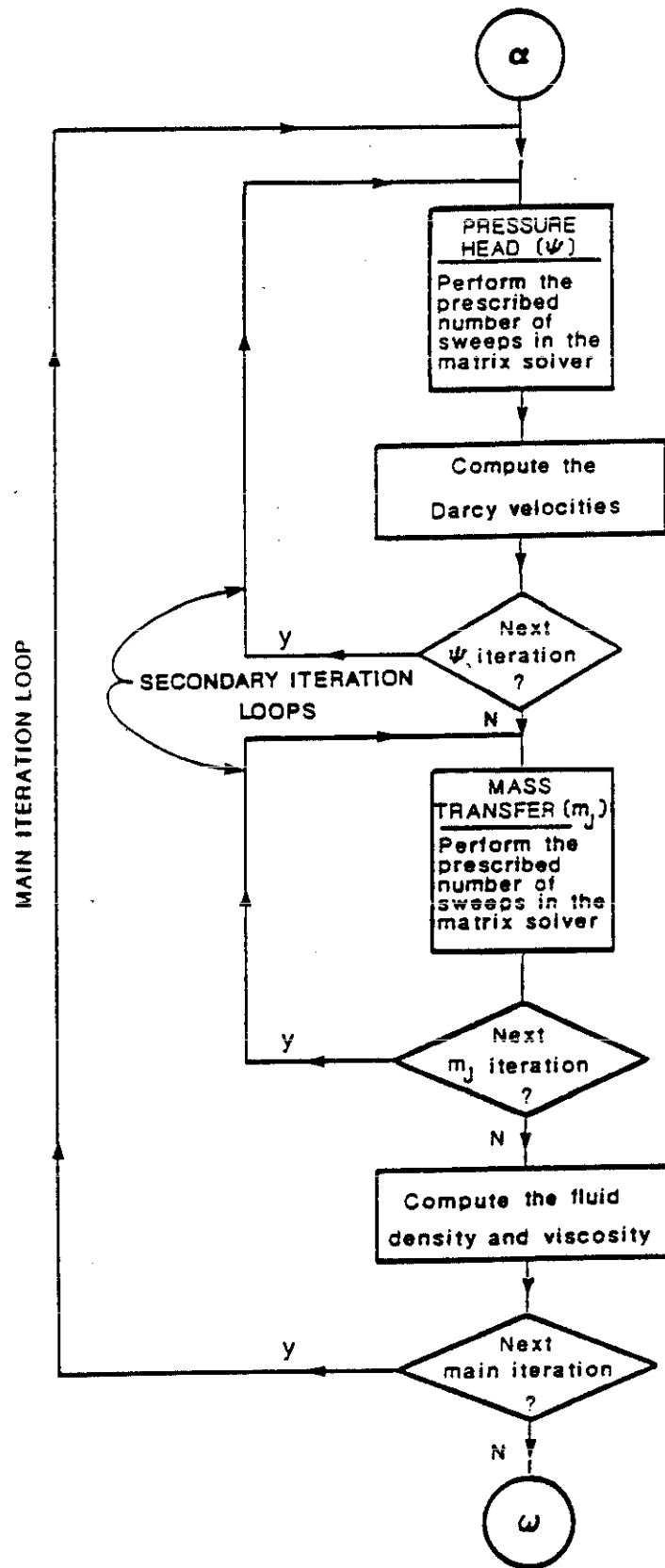


Figure A-3. Iteration scheme.

when the correction is everywhere identical to zero. Due to the nonlinear nature of some of the coefficients in the fundamental equations, the convergence rate can show strong variations from one problem to another. To accelerate or damp the convergence rate, the correction is multiplied by a relaxation factor before being added to the primary variable.

Density coupled problems are inherently unstable because variations in fluid densities affect the solution of the pressure head equation. To stabilize this effect, an additional relaxation factor has been introduced in the density term itself. This approach has enabled simulation of otherwise intractable problems.

VALIDATION CASES

Three validation cases are illustrated on the following pages. They have been chosen to illustrate a range of model features as well as a variety of types of validation.

One-Dimensional Transport: Comparison with Analytical Solution

The first case considered involves uniform flow in one dimension subject to the introduction of a contaminant of constant concentration. The distribution of contaminant concentration along the direction of flow, with time, is investigated.

The initial and boundary conditions are

x = distance along the direction of flow

C = tracer concentration for time = $\begin{cases} t \leq 0, C = 0 & \text{at } x = 0 \\ t > 0, C = C_0 & \text{at } x = 0 \end{cases}$

u = velocity = 1 ft/d

D = dispersion coefficient = 1 ft²/d.

The exact analytical solution to this problem (Freeze and Cherry 1979) is

$$\frac{C}{C_0} = \frac{1}{2} \left[\operatorname{erfc} \left(\frac{x - ut}{2\sqrt{Dt}} \right) + \exp \left(\frac{ux}{D} \right) \operatorname{erfc} \left(\frac{x + ut}{2\sqrt{Dt}} \right) \right]$$

The finite-difference grid consists of 100 cells 10-ft long, for a total soil column of 1,000 ft.

The analytical solution and predicted results are shown in Figure A-4. The simulated concentration distributions compare favorably with the exact solution.

Two-Dimensional, Variably-Saturated Flow: Comparison with Laboratory Data

In this validation case, transient drainage from a sandbox involving transition from saturated to unsaturated conditions was considered. The experiment setup involved a sandbox filled with fine, homogeneous sand, saturated to a depth of 1.43 m. The movement of the free surface was investigated with one end of the sandbox maintained at a constant head and the other end allowed to drain (Vachaud et al. 1971, Vauclin et al. 1975). The experiment setup and unsaturated hydraulic parameter characteristics are shown in Figure A-5.

The model simulation used a finite-difference grid with 32 cells in the horizontal direction and 31 cells in the vertical direction. The cells ranged in size from 1 cm by 1 cm to 24 cm by 16 cm with the smaller cells concentrated in the area of drainage and varying pressure head.

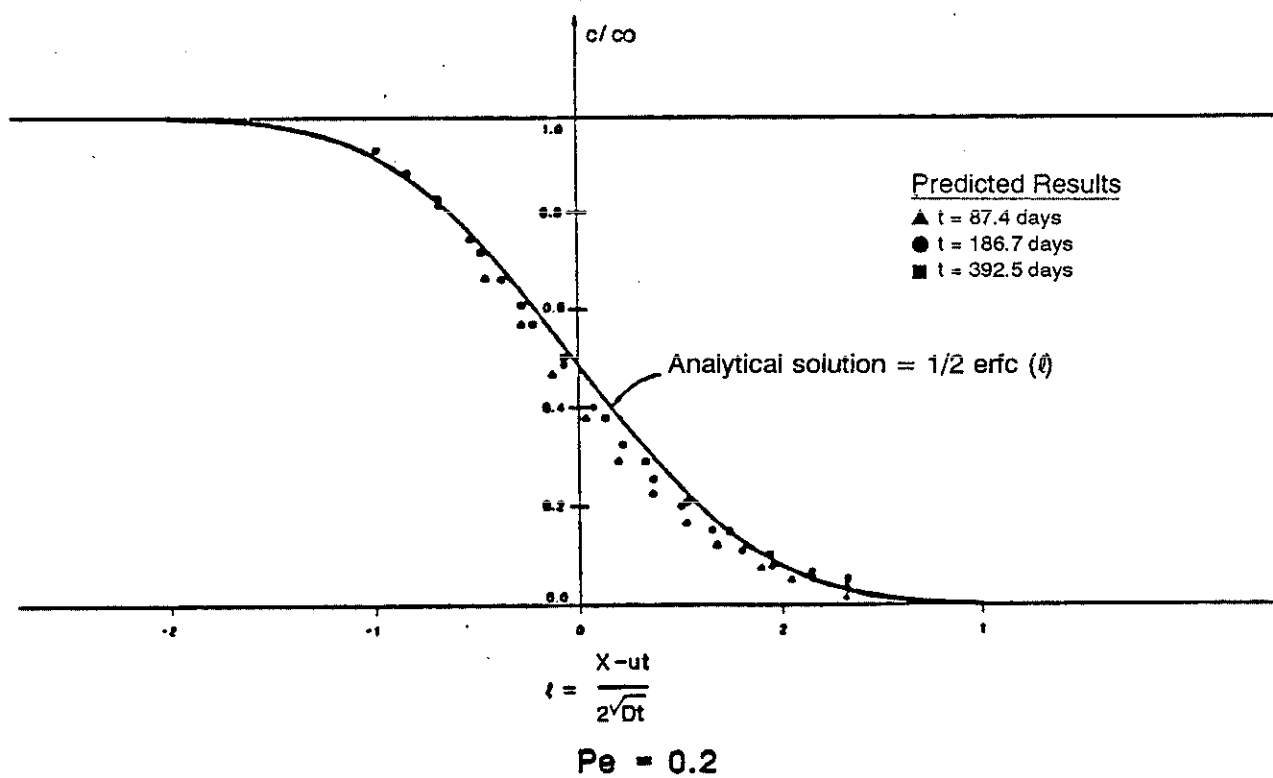
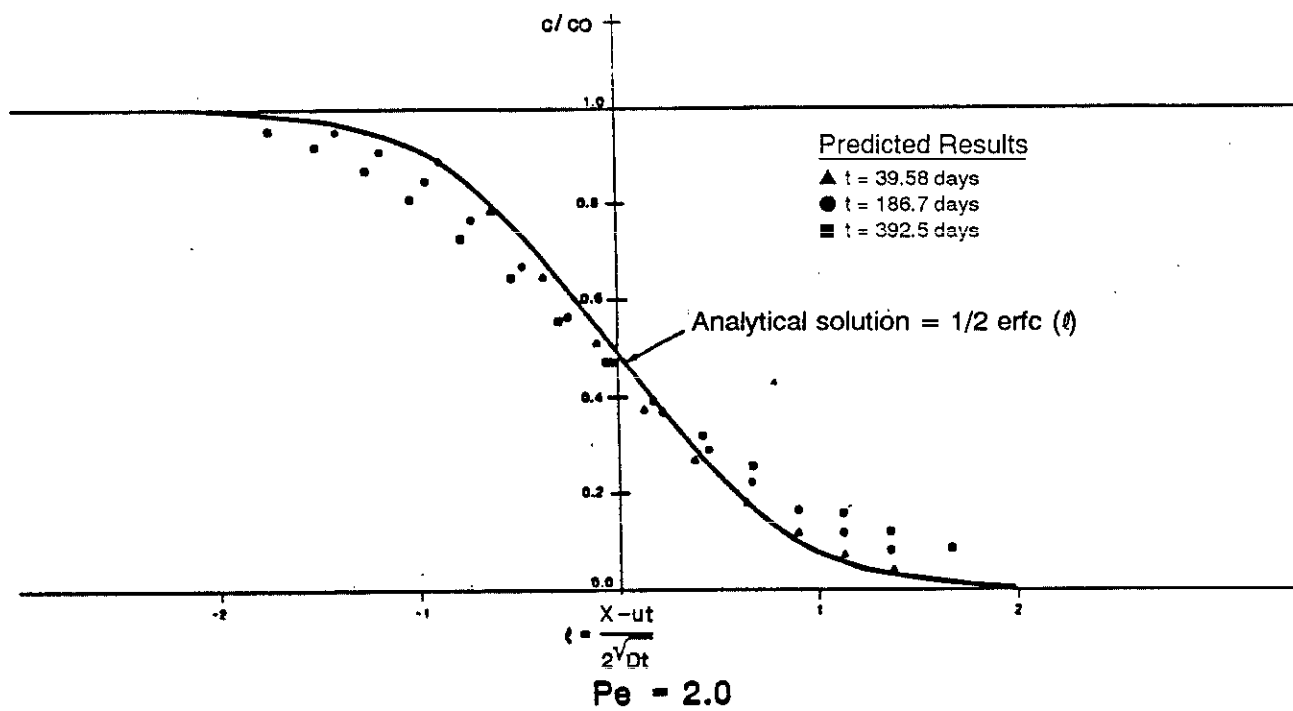
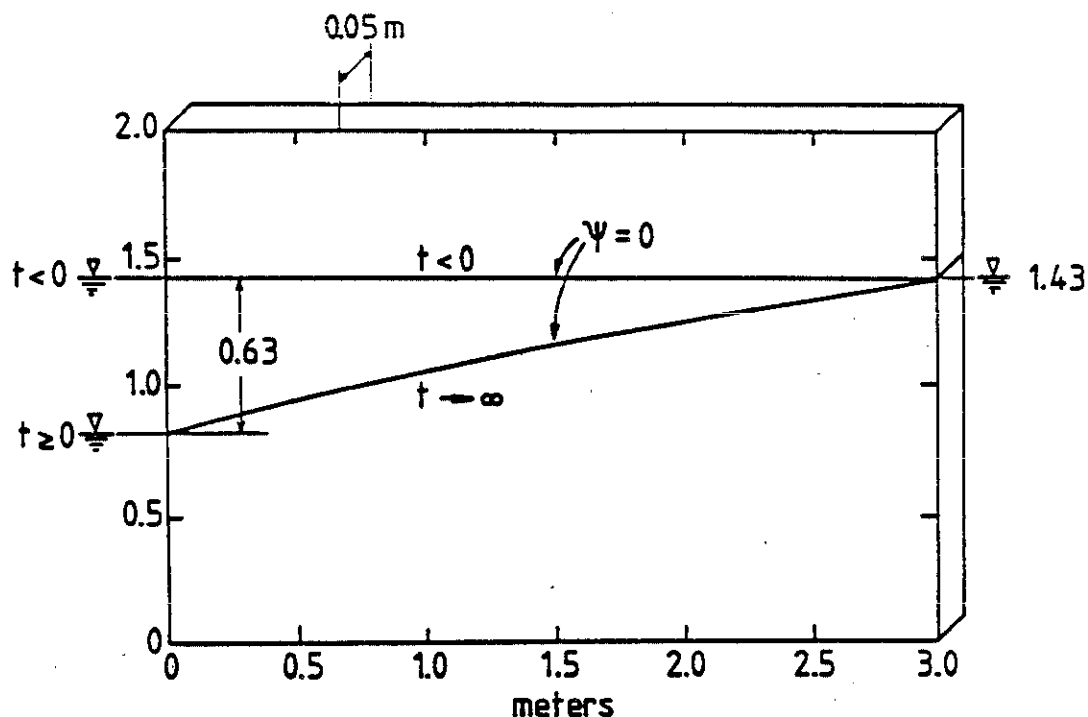


Figure A-4. One-dimensional transport solutions.



EXPERIMENTAL SETUP
FALLING WATER TABLE SIMULATION

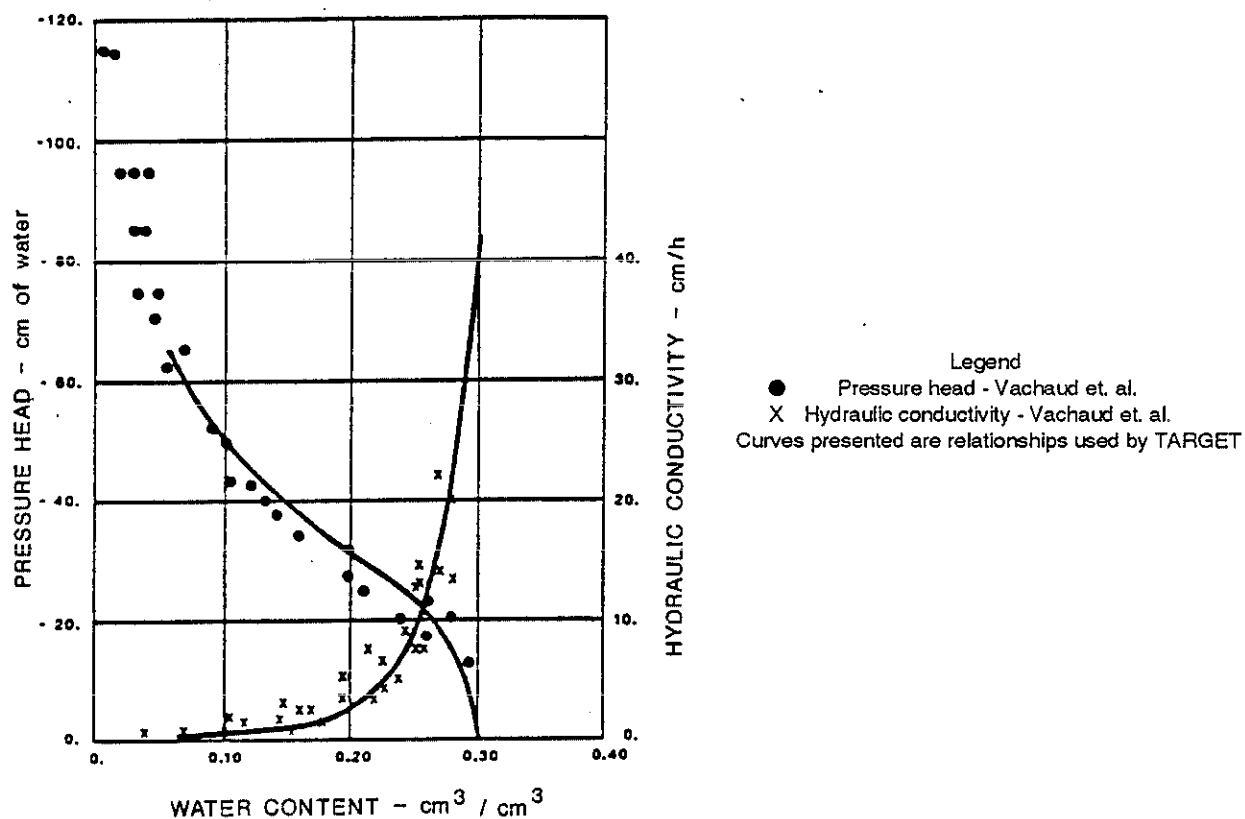


Figure A-5. Comparison of TARGET model representation and experimentally obtained data.

Other parameters supplied to the model include the following:

x-direction hydraulic conductivity = 0.011 cm/s

z-direction hydraulic conductivity = 0.011 cm/s

storativity = 4.9×10^{-5}

porosity = 0.3

The model prediction of the location of the free surface at various times is plotted in Figure A-6. The experimentally-obtained data are also presented in these figures. The modeled results are in good agreement with the laboratory data.

Two-Dimensional, Transient Flow: Comparison with Numerical Model

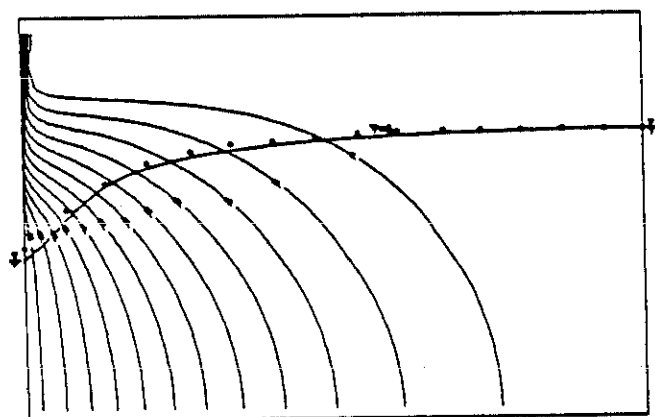
This validation case resulted from an actual Dames & Moore project (Dames & Moore 1983b). The model was used to predict the hydraulic head distribution in the area of the Jackpile-Paguate Uranium Mine in New Mexico before and after mining activities. The results were used to recommend the degree of backfilling necessary to reclaim the mined area and restore the water table to conditions similar to its original, natural state. The long-term effects of the backfilling efforts on water table recovery were predicted.

Following Dames & Moore's modeling analyses using the TARGET model, the USGS also modeled the problem. They used their generic, two-dimensional groundwater flow model. The results of these two modeling efforts are compared in this case.

The Jackpile-Paguate Mine is comprised of three major open pits and a major underground mine. The mine is located in an area of rough and broken terrain ranging in elevation from 5,700 to 7,000 ft. The topographic features are characterized by broad mesas and plateaus interspersed with deep canyons, dry washes, and broad valleys. Little pre-mining groundwater data were available for the area. Estimated pre-mining contours of groundwater elevation were also developed for the project using the TARGET model. Groundwater in the area is confined, except locally near open pits and outcrops. The input parameters supplied to the model by Dames & Moore are presented below. These parameters were also used by USGS.

The finite difference grid consisted of 42 cells in the east-west direction and 34 cells in the north-south direction. The cell sizes ranged from 500 ft by 500 ft to 6,000 ft by 8,000 ft. The smaller cells were concentrated in the area of the mine pits. The north, east, and west edges of the model domain were set as zero flux (impermeable) boundaries. Recharge to the system was simulated by a constant flux over a large areal portion of the aquifer.

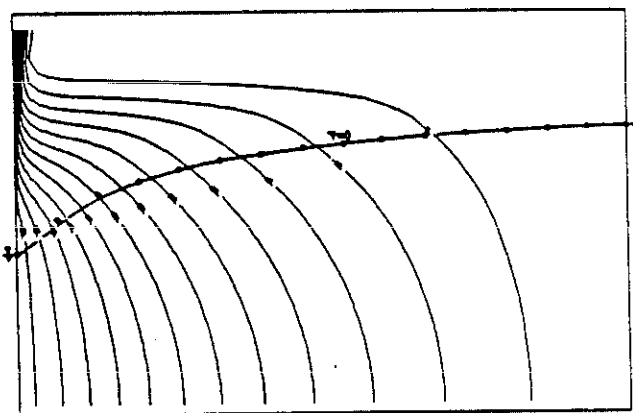
The thickness of the Jackpile sandstone was input to the model on a cell-by-cell basis based on a detailed map showing thickness of the unit at several hundred drill hole sites. The hydraulic



POTENTIAL HEAD (H)

© VACHAUD, et al.

Plot Time = 108 Step = 17



conductivity varied from cell to cell in the model based on observed conditions. The values supplied to the model varied from 0.05 to 22 ft/d, except for backfill material, which was assumed to have a conductivity of 190 ft/d.

The storage coefficient for confined conditions in the Jackpile sandstone was modeled based on a specific storage of 2.5×10^{-6} ft⁻¹ and the local thickness of the aquifer. For unconfined conditions, a specific yield of 0.20 was used. Total porosity of the Jackpile sandstone was estimated at about 28% based on an in situ density of 120 lb/ft³. Total porosity of the backfill was estimated at 45%. Recharge to the aquifer was estimated to range between 0.12 to 0.24 in./yr. The total recharge rate to the model was 12,700 ft³/d (66 gpm).

The USGS modeling effort varied from the Dames & Moore effort in two ways: (a) cells in outcrop areas were permitted to completely desaturate, and (b) the larger cells in the finite-difference grid were split into two cells to increase numerical stability in the USGS model.

As can be seen in Figures A-7 through A-9, the results from simulating the mine pit backfilling in each model are consistent. In the simulation of the pre-mining case, the predicted heads from the two models are generally within 5 ft. For the post-mining simulations, the results also agree closely except in the vicinity of the outcrop of the aquifer, where the USGS model computes heads that are commonly more than 40 ft higher than the TARGET model. These discrepancies diminish rapidly with distance from the outcrop.

In performing a comparison between the two modeling efforts, USGS stated that they found "no inconsistencies of a mathematical or programming nature which significantly affected its results" when discussing the TARGET model.

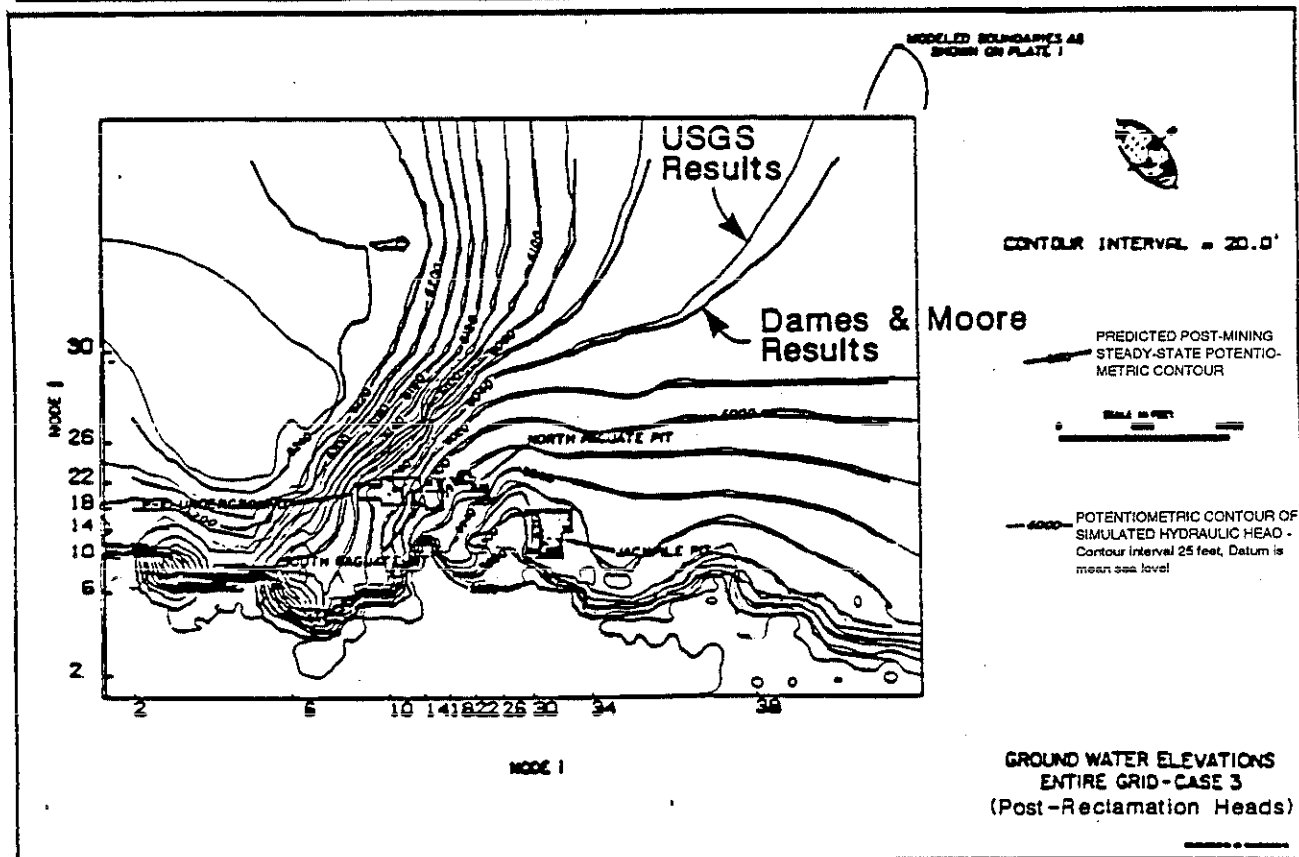
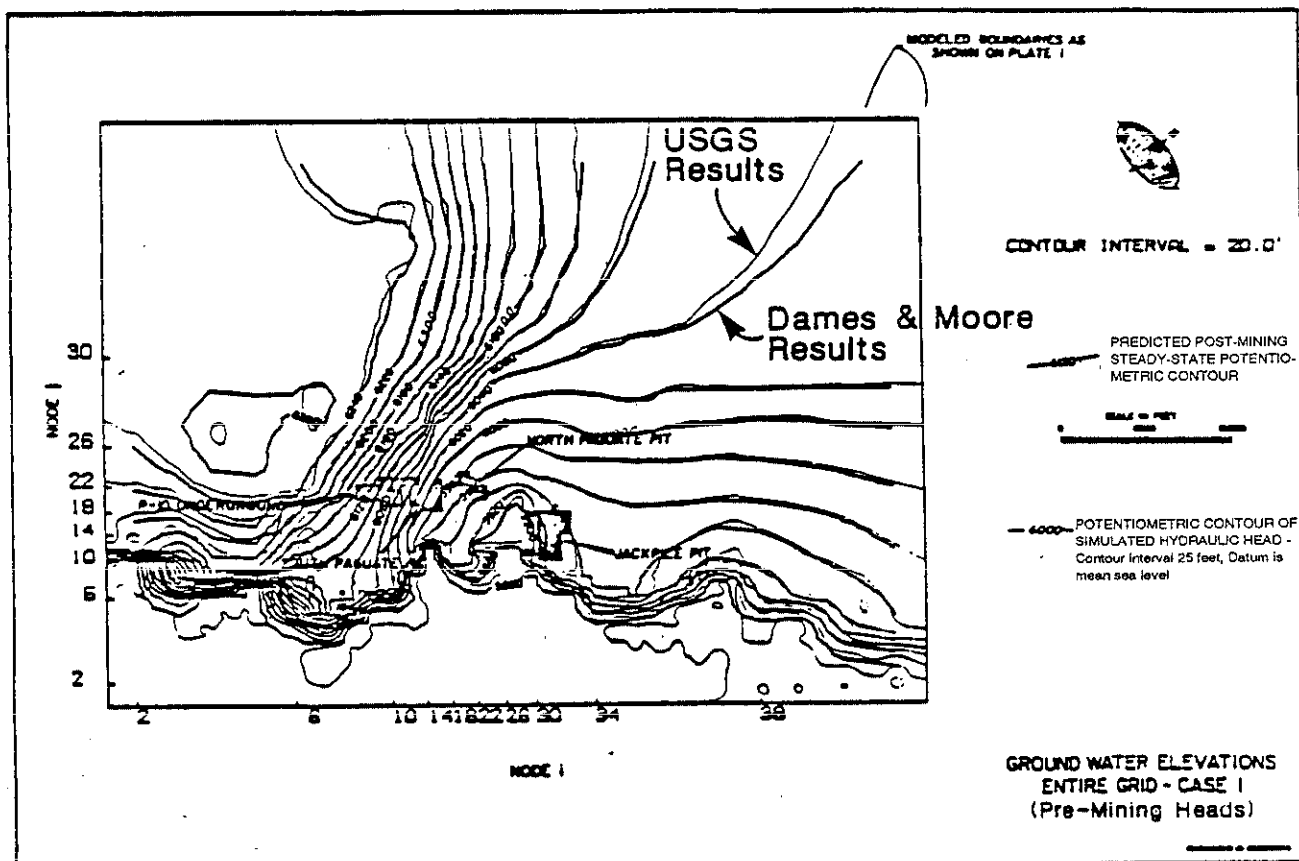


Figure A-7. Comparison of model predictions for the entire grid of pre-mining and post-reclamation heads.

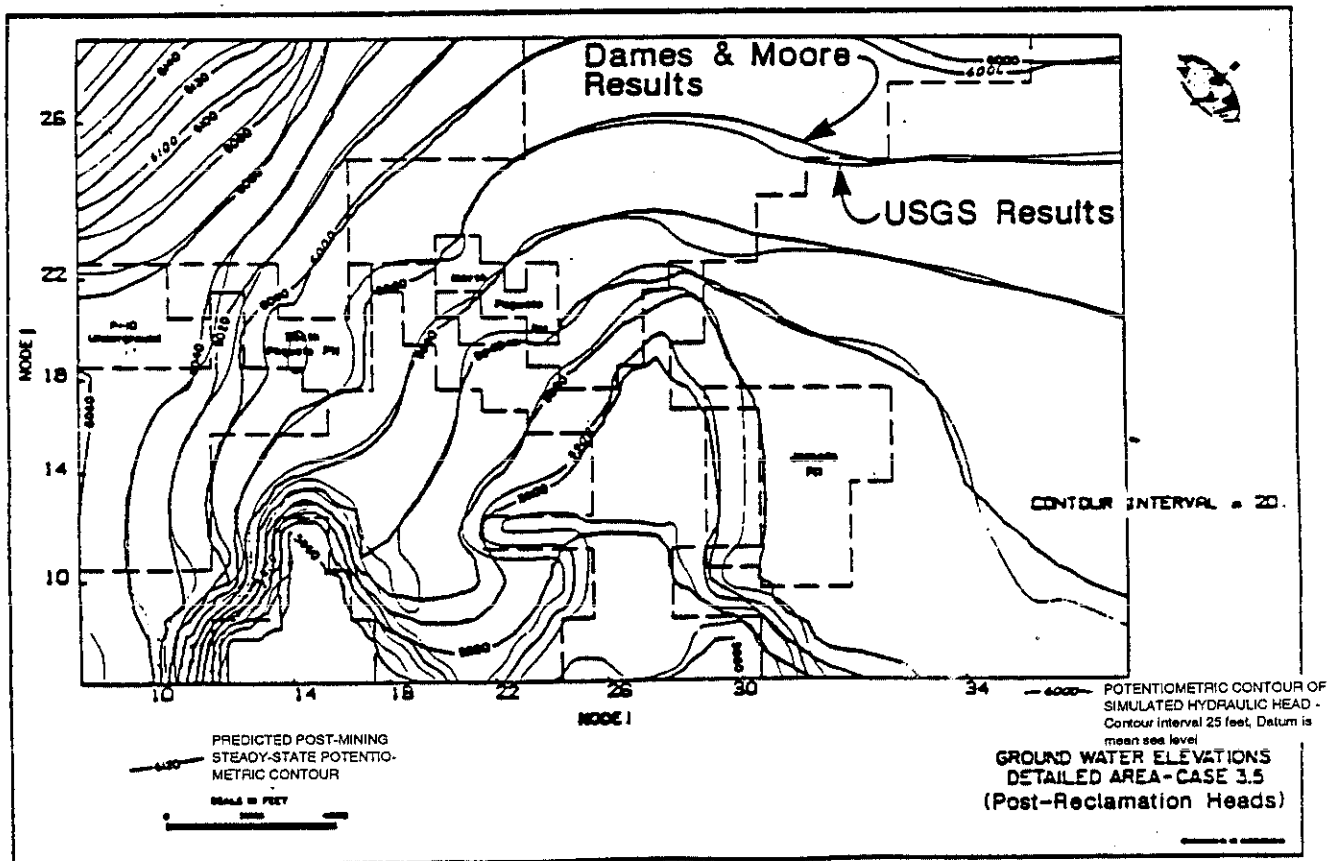
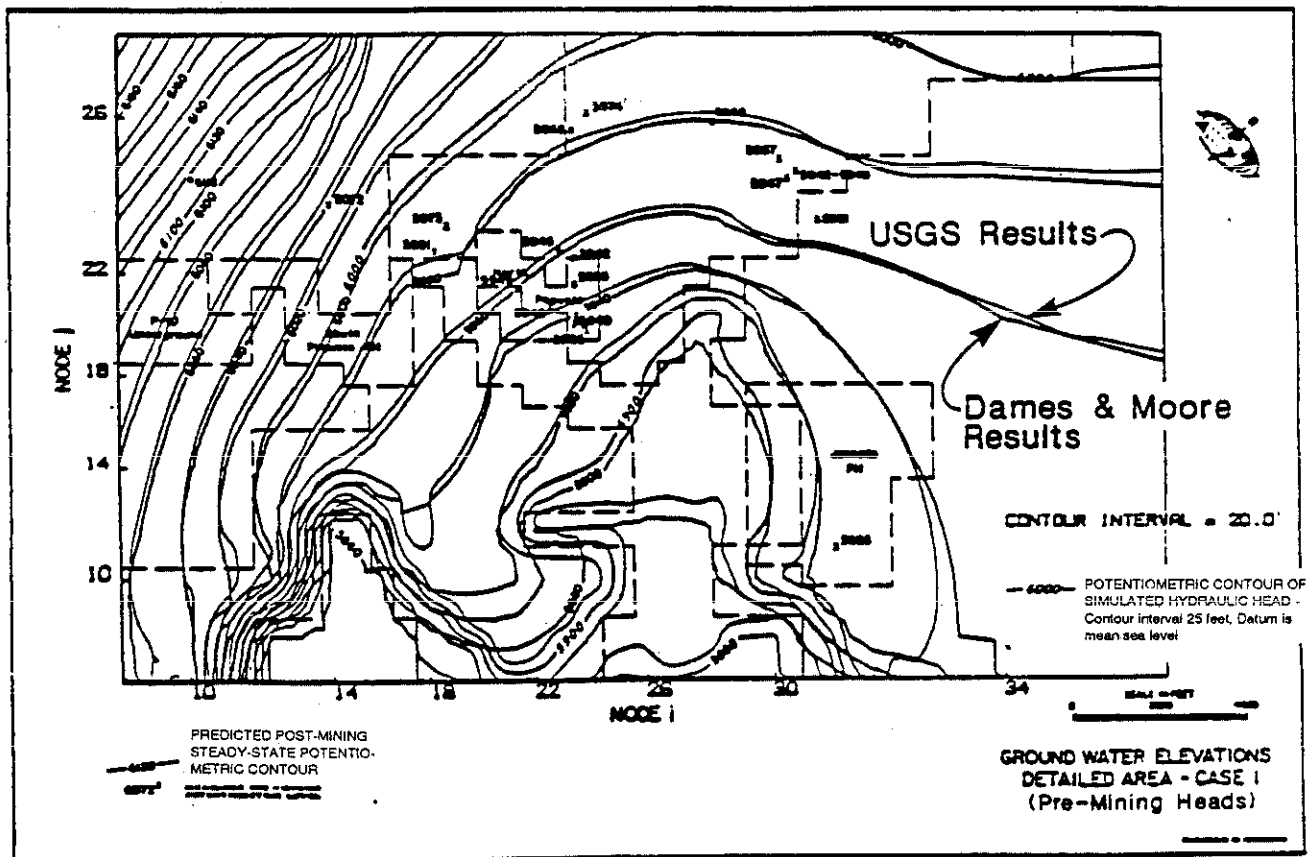


Figure A-8. Comparison of model predictions for the detailed area of pre-mining and post-reclamation heads.

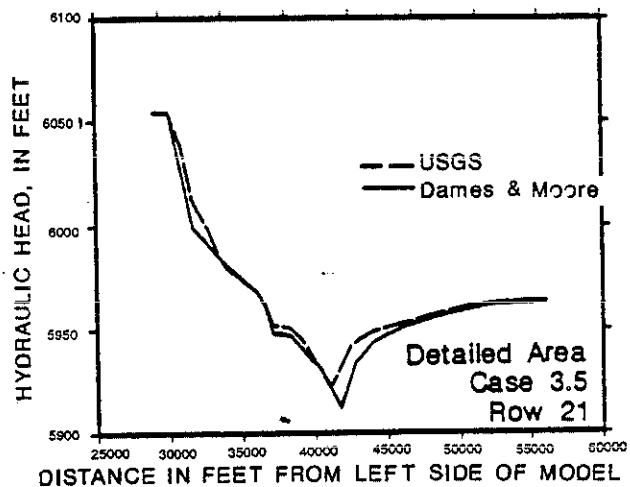
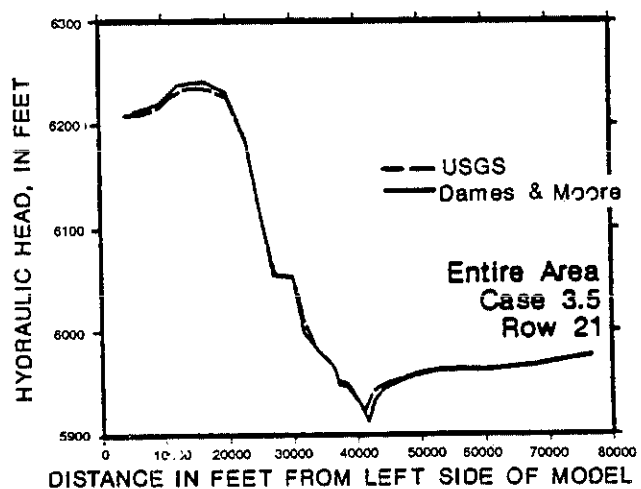
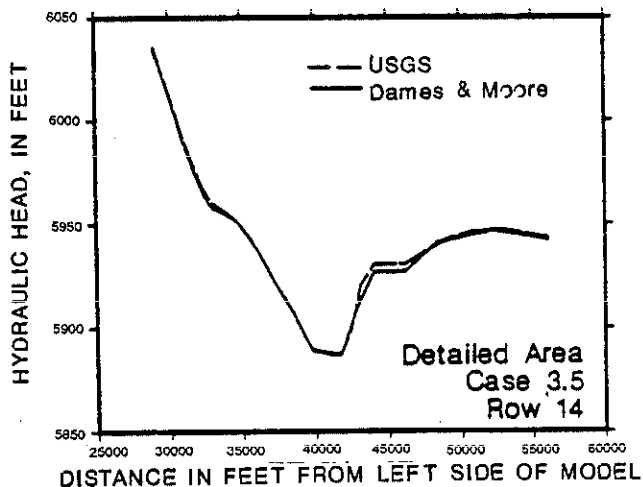
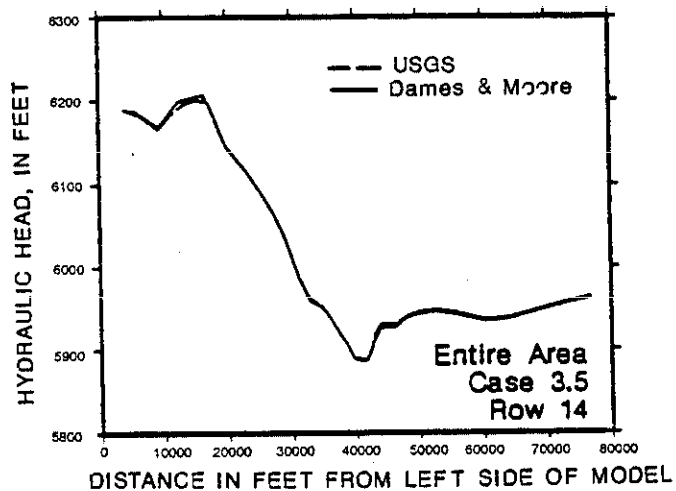


Figure A-9. Comparison of the USGS and Dames & Moore model predictions for several cross sections.

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Appendix B

Peer Review Report on the TARGET Models by Professor R. Allan Freeze

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Peer Review Report on the TARGET Models by Professor R. Allan Freeze

July 10, 1985

Dr. D. A. Stephenson
Dames & Moore
2727 N. 7th Street, Suite 121
Phoenix, Arizona
U.S.A. 85014

Dear Dave:

In response to your letter of June 11, 1985, I reviewed the Dames & Moore TARGET package, giving special considerations to the suitability of the documentation for outside-the-firm release. I have divided my comments into general comments and specific comments.

GENERAL COMMENTS

1. It is clear to me that the TARGET package is a versatile and powerful set of computer programs for the mathematical modeling of groundwater flow and solute transport. The mathematical foundations are strong and the numerical methodology clever and efficient. It is clear that the authors of the program and the documentation are working from a strong technical base.
2. The writing style throughout the report is very clear. I will have some comments about the level and order of presentation, but I must emphasize that the current presentation of each topic, both in their descriptive and mathematical contexts, is very well done.
3. The major area of concern that I can identify lies in the level of sophistication in the chapter on the Physical and Mathematical Background of the models. This chapter uses a very sophisticated mathematical framework and a very advanced notation. As a research scientist in this field I find it compact and elegant, but my experience in dealing with small consulting firms who may provide a primary market for TARGET would lead me to question whether engineers from such firms would be at home with this level of presentation. One must ask to whom this chapter is directed. If it is directed to reviewers such as myself as a kind of base document that lays out the mathematical foundations of the programs for those few who may wish to follow it up, then the current presentation may be suitable. If, on

the other hand, it is intended as a kind of textbook to accompany training sessions for consulting engineers from smaller companies, then I believe it needs to be expanded and the order changed somewhat in order to bring it into line with the backgrounds that such "students" will have. Several of the Specific Comments pertain to this issue, but the more general suggestions are as follows:

- (a) The Introduction should be expanded to include more complete descriptions of the types of boundary-value problems that the programs can handle (and the engineering problems to which they apply). It should include clear definitions of such concepts as steady-state and transient flow, unsaturated and saturated pressure heads, homogeneity and anisotropy, etc.
- (b) Section 2-0 on Physical Mechanisms and Chemical Processes should include detailed positive statements of the capabilities of the models with respect to ground-water flow and solute transport. In the current write-up the basic assumptions of Section 2-1-1 hit the reader without lead in or warning. Some of them are quite sophisticated and required a detailed understanding of the equations of ground-water flow. I would be inclined to save this list until after the primary development of Section 3-0.
- (c) The references provided in the Introduction are a bit obscure. I would refer to the available textbooks by Wang and Anderson, Pinder and Gray, Remson et al, and to the AGU monograph by Bredehoeft et al and the NWWA monograph by Mercer and Faust.
- (d) Much of the descriptive material is too terse. Two examples: (i) Section 2-2 on Solute Transport ought to summarize all the mechanisms of transport noting which ones are included and which ones are not; (ii) The discussion of seepage faces in the 2nd paragraph from the bottom of page 16 does not hint at the complexities associated with their simulation (iterative positioning of the exit point, problems associated with multiple seepage faces, etc.).
- (e) There are many examples in the Specific Comment of cases where the readers first encounter with a concept or notation occurs in the midst of some other explanation. Examples: (i) on p. 26 just below Eqn. (4-38) the reader is first informed that the numerical solution is iterative; (ii) the Peclet number is introduced for the first time on page 3-1 in the Validation Chapter. In all cases, introductory material should have appeared earlier so that the reader is not taken by surprise.
- (f) I would prefer to see variables defined at the point of first encounter as well as in the notation list. It is difficult for the reader to switch back and forth from the text to the list and to locate the particular symbol on the list.

4. In the Introduction it is stated that there are 5 models in the TARGET family, but there are 18 possible combinations of the properties listed there. The 5 models should be identified clearly and examples of their use described. Model TARGET_2DH does not figure anywhere in the Background chapter or the User's Guides, but it appears in the first two validation cases.
5. The User's Guide to TARGET_2DU and TARGET_3DS are clearly done and should prove easy to follow by prospective clients. The Specific Comments note a few places where clarification is needed. I note, however, that a list clearly relating the computer acronyms to their mathematical notation in the Background chapter would be useful.
6. The chapter on the Summary of Validation Cases is clear and convincing. The only apparent capability of the TARGET family that is not fully validated is a case that involves solute transport in the unsaturated zone. If such a validation is available, it would make a worthwhile addition.*

*Note from Dames & Moore: Subsequent to Professor Freeze's review a validation case for unsaturated flow and transport has been conducted, and now forms part of the model documentation.

Appendix C

Selected TARGET Validation Cases

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Selected TARGET Validation Cases

CASE 7: TARGET 2DH VALIDATION—COMPARISON WITH USGS MODEL

Mine Pit Backfilling Investigation Generated March 1983

Objective

This validation case resulted from an actual Dames & Moore project (Dames & Moore 1983). The model was used to predict the hydraulic head distribution in the area of the Jackpile-Paguate Uranium Mine in New Mexico before and after mining activities. The results were used to recommend the degree of backfilling necessary to reclaim the mined area and restore the water table to conditions similar to its original, natural state. The long-range effects of the backfilling efforts on water table recovery were predicted.

Following Dames & Moore's modeling using the TARGET model, the U.S. Geological Survey (USGS) also modeled the problem with their generic, two-dimensional groundwater flow model (USGS 1984). The results of these two modeling efforts are presented in this case.

Description

The Jackpile-Paguate Mine is comprised of three major open pits and a major underground mine. The mine is located in an area of rough and broken terrain ranging in elevation from 5700 to 7000 ft. The topographic features are characterized by broad mesas and plateaus interspersed with deep canyons, dry washes, and broad valleys. Two major surface streams flow in the vicinity of the mine. As part of the proposed reclamation plan, open pit mines are to be backfilled to an elevation 3 ft above the anticipated post-reclamation water table recovery elevation. Modeling was used to estimate the maximum probable recovery elevation of the water table in the pits.

Little pre-mining groundwater data were available for the area. Estimated pre-mining contours of groundwater elevation were also developed for the project using the TARGET model. Except locally near open pits and outcrops, groundwater in the area is confined.

Specification

The input parameters supplied to the model by Dames & Moore are presented below. These parameters also were used by USGS to the extent possible to maximize the similarity of the modeled conditions.

The finite difference grid used consisted of 42 cells in the east-west direction and 34 cells in the north-south direction. The cell sizes ranged from 500 ft by 500 ft to 6,000 ft by 8,000 ft. The smaller cells were concentrated in the area of the mine pits.

The upper boundary of the model, the left boundary, and the right boundary all were set as zero flux (impermeable) boundaries. To simulate the outcrop of the Jackpile Sandstone and its contact with alluvium along the Rio Paguete and Rio Moquino (the two major streams), an area of high hydraulic conductivity was placed along the lower portion of the grid and a fixed head was placed along the lower edge of the grid. A fixed head was also placed at the upper reach of the Rio Paguete alluvium to simulate the interconnection of the Rio Paguete and Rio Moquino surface streams along the extent of the alluvium. The fixed head was set at an appropriate elevation in two nodes to simulate groundwater levels in alluvium along the Rio Paguete and its uppermost interconnection with the Jackpile Sandstone. By fixing the heads in these nodes, groundwater levels in nodes representing alluvium downgradient closely approximate those encountered in the field. Recharge to the system was simulated by a constant flux over a large areal portion of the aquifer. This combination of boundary conditions allows simulation of groundwater flow from recharge areas to outcrop areas.

The thickness of the Jackpile Sandstone was input to the model on a cell-by-cell basis based on a detailed map showing thickness of the unit at several hundred drill hole sites. The combination of saturated thickness and hydraulic conductivity of the Jackpile Sandstone was used in the model to estimate transmissivity on a cell-by-cell basis.

The hydraulic conductivity varied from cell to cell in the model based on actual conditions. The values supplied to the model varied from 0.05 to 22 ft/d except for backfill material, which was modeled as 190 ft/d.

The storage coefficient for confined conditions in the Jackpile Sandstone was modeled based on a specific storage of 2.5×10^{-6} ft⁻¹ and the local thickness of the aquifer. For unconfined conditions, a storage coefficient (specific yield) of 0.20 was used in the model. Total porosity of the Jackpile Sandstone was estimated at about 28% based on an in situ density of 120 lb/ft³.

Total porosity of backfill was estimated at 45%. The initial volumetric moisture content was measured at approximately 15%. Therefore, an unconfined storage coefficient of 0.30 was used in the model. The backfill is never under confined conditions and, therefore, a confined storage coefficient is not required for the backfill material. Virtually no changes occur in water levels in alluvium; therefore, the model is insensitive to the values chosen for storativity of the alluvium.

Recharge to the aquifer was estimated to range between 0.12 and 0.24 in./yr. The total recharge rate to the model was 12,700 ft³/d (66 gpm).

The numerical solutions used by the USGS and Dames & Moore models are different. Therefore, two modifications were made to the USGS model to perform modeling comparable to that of Dames & Moore. First, the TARGET model requires that all cells (including the perimeter boundary) have a finite transmissivity. The USGS model was modified to match the TARGET model's requirement of minimum transmissivity based on an equivalent thickness of 0.10 ft of saturated aquifer.

The second modification concerns the treatment of the modeled outcrop boundary. The TARGET model's requirement that cells have a finite transmissivity causes a small, steady groundwater flow through outcrop areas. This treatment was abandoned in the USGS model to allow cells to completely desaturate. This change allowed a steady-state simulation to be completed and further improved the agreement between the models for the simulated pre-mining steady-state hydraulic head distribution.

The USGS modeling effort also varied from the Dames & Moore effort in its simulation of field conditions in the model. The larger cells in the finite-difference grid were split into two cells to increase numerical stability in the USGS model.

Results

The results of the model comparisons are presented in Figures C-1 through C-9. Three scenarios are represented in these figures and are labeled as follows:

Case 1—Pre-mining simulation

Case 2—Post-mining simulation

Case 3.5—Post-mining simulation with recommended in-pit dam installed.

The figures present comparisons over the entire modeled area, the immediate mine area, and cross sections along selected grid rows through the mine area.

Discussion

As can be seen in the accompanying figures, the results of simulation of the mine pit backfilling presented herein are consistent. In the simulation of the pre-mining case, the results from the two models are generally within 5 ft in computed heads. For the post-mining simulations, the results also agree closely except in the vicinity of the outcrop of the aquifer, where the USGS model computes heads that are commonly more than 40 ft higher than the TARGET model. These discrepancies diminish rapidly with distance from the outcrop.

In performing the comparison, USGS stated in the discussion of their report that they found "no inconsistencies of a mathematical or programming nature which significantly affected its results" when discussing the TARGET model.

References

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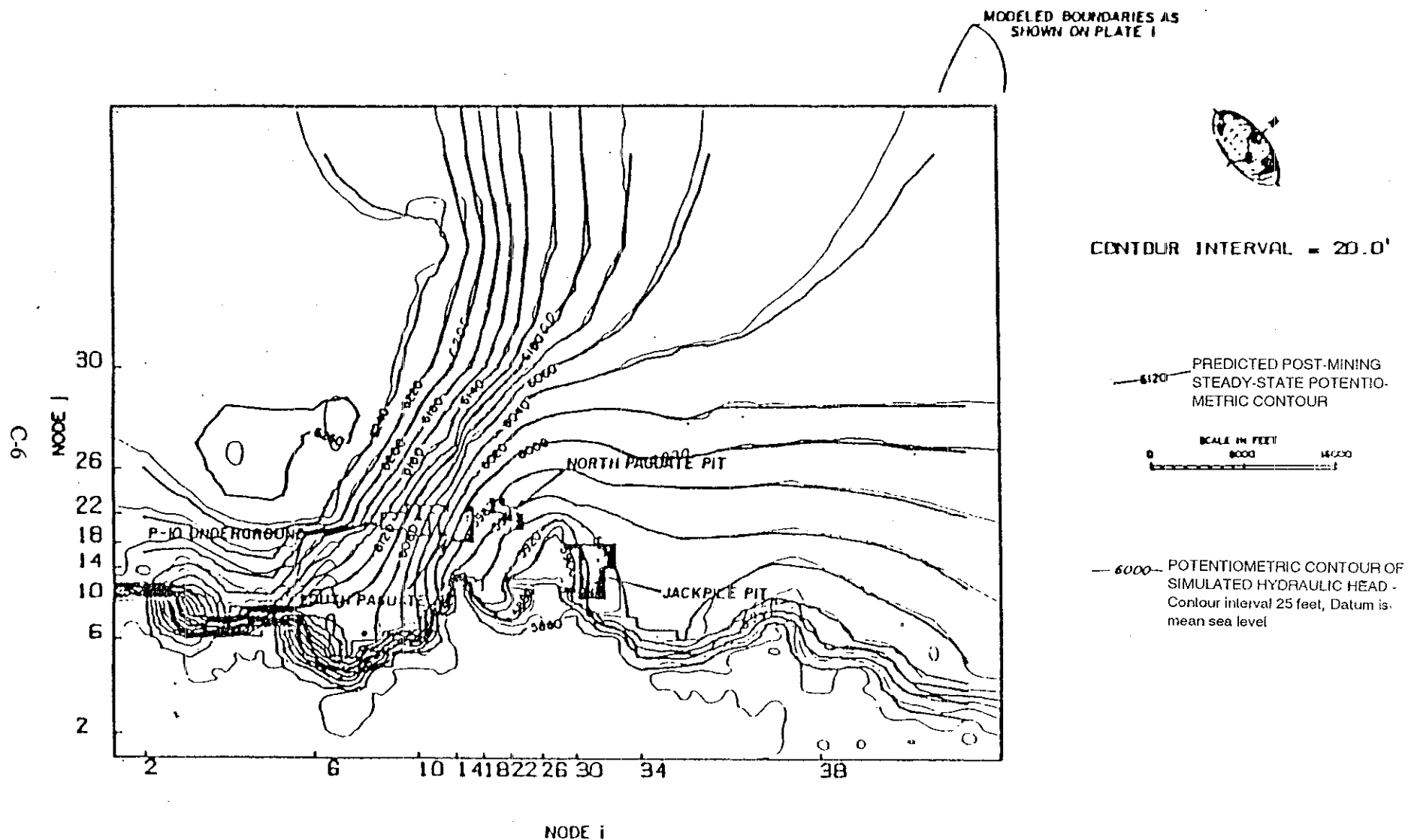


Figure C-1. Simulated pre-mining potentiometric heads in the entire modeled area for Case 1.

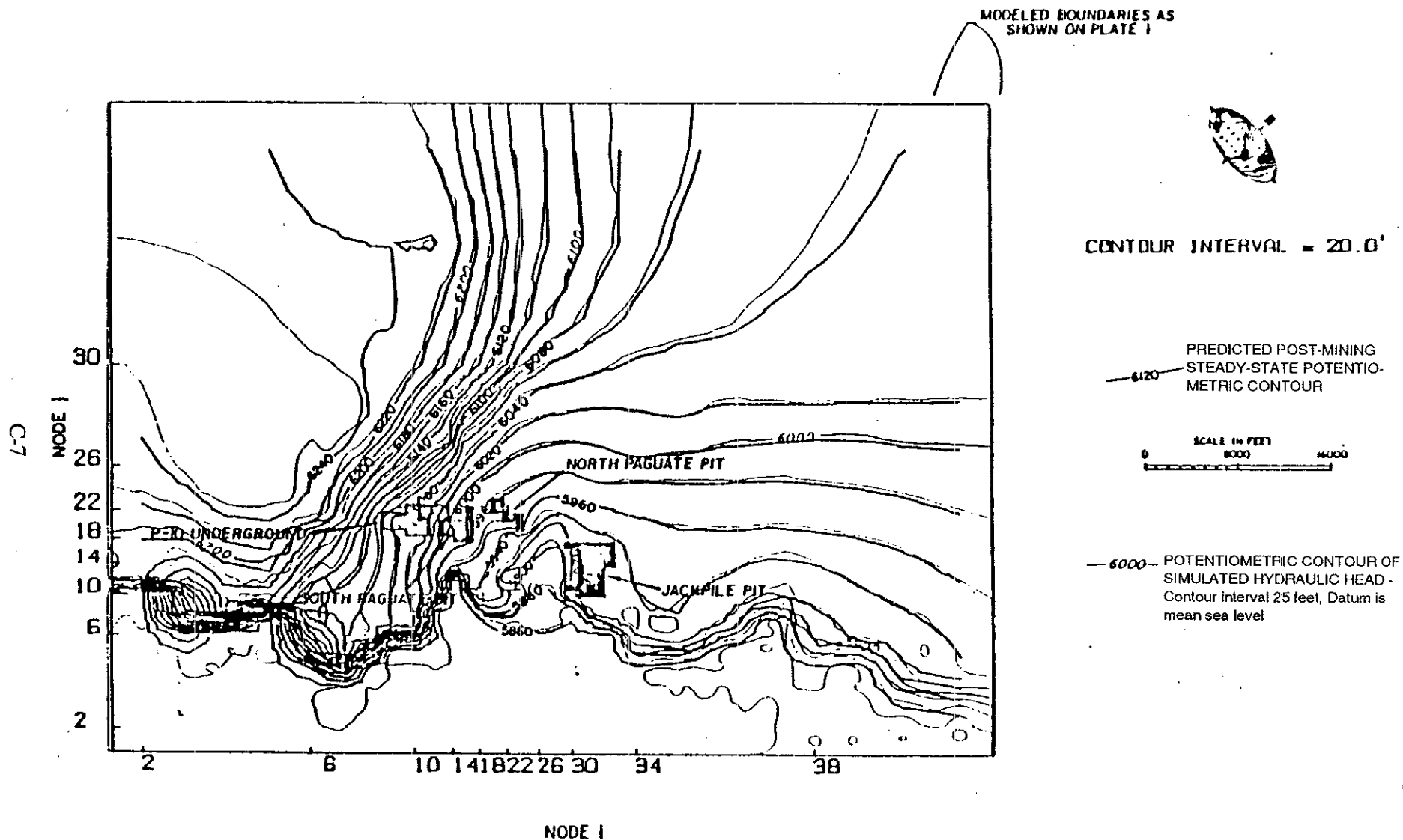


Figure C-2. Simulated post-mining and post-reclamation potentiometric heads (without artificial hydraulic barrier) in the entire modeled area for Case 3.

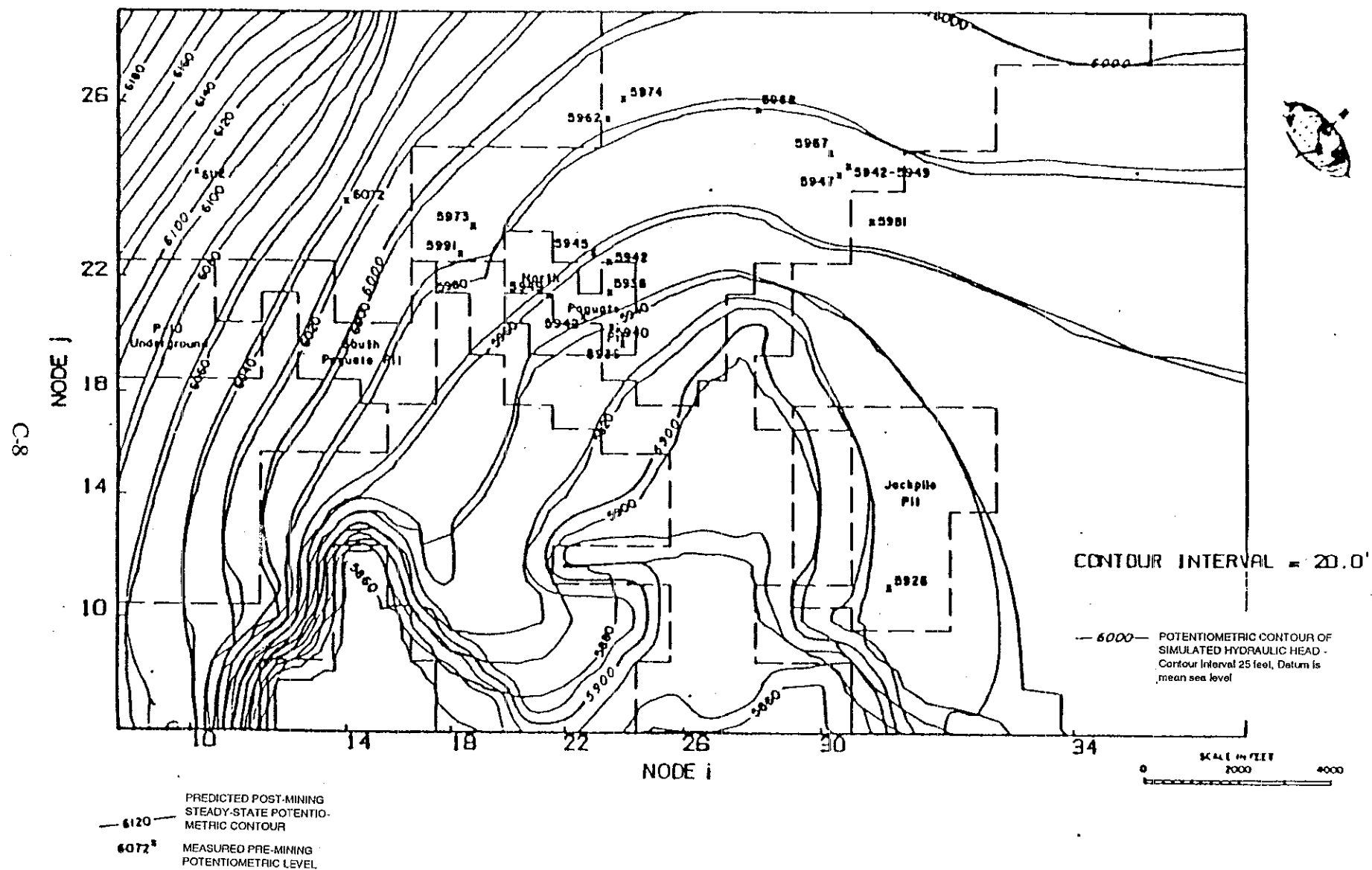


Figure C-3. Simulated pre-mining potentiometric heads in the immediate mine area for Case 1.

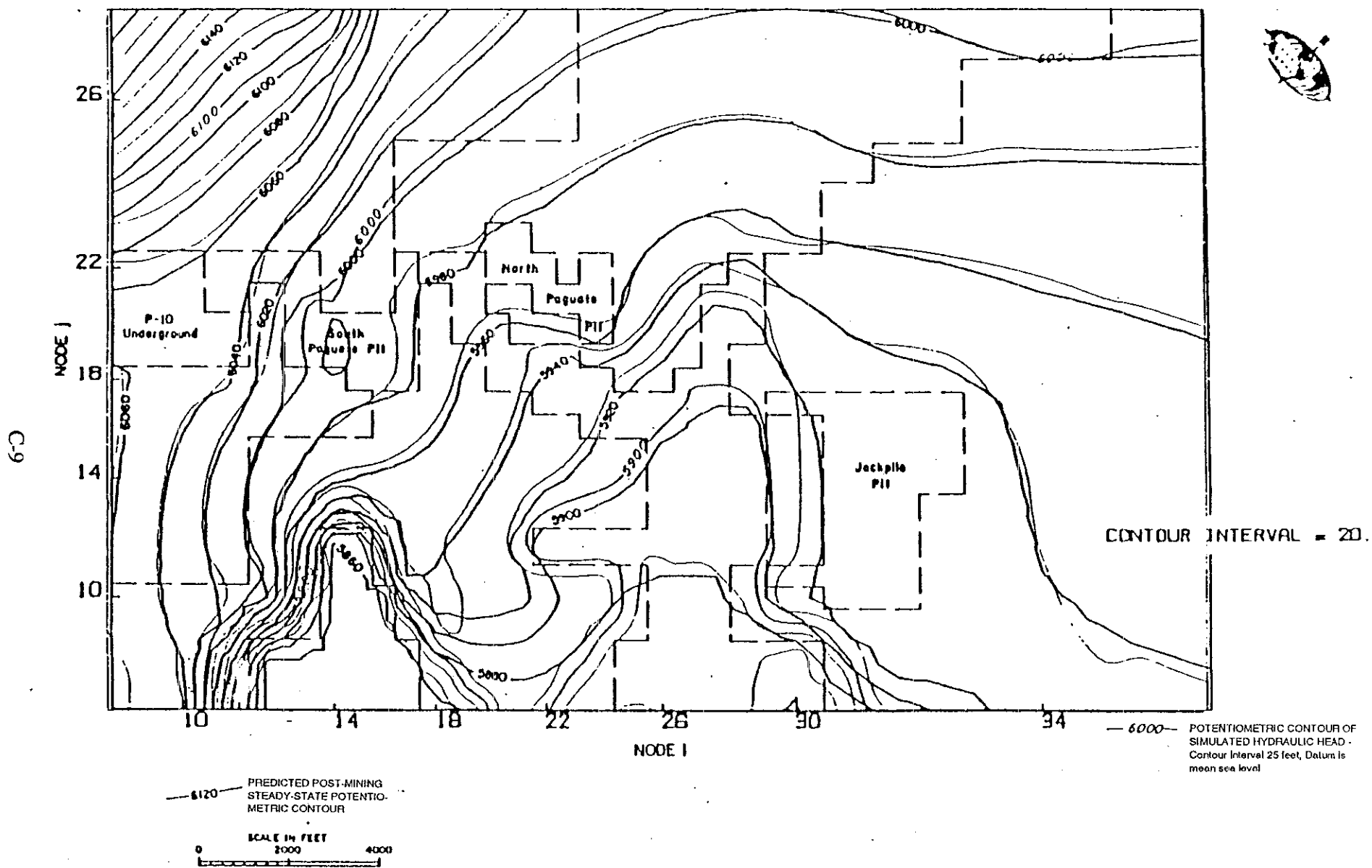


Figure C-4. Simulated post-mining and reclamation potentiometric heads (without artificial hydraulic barrier) in the immediate mine area for Case 3.

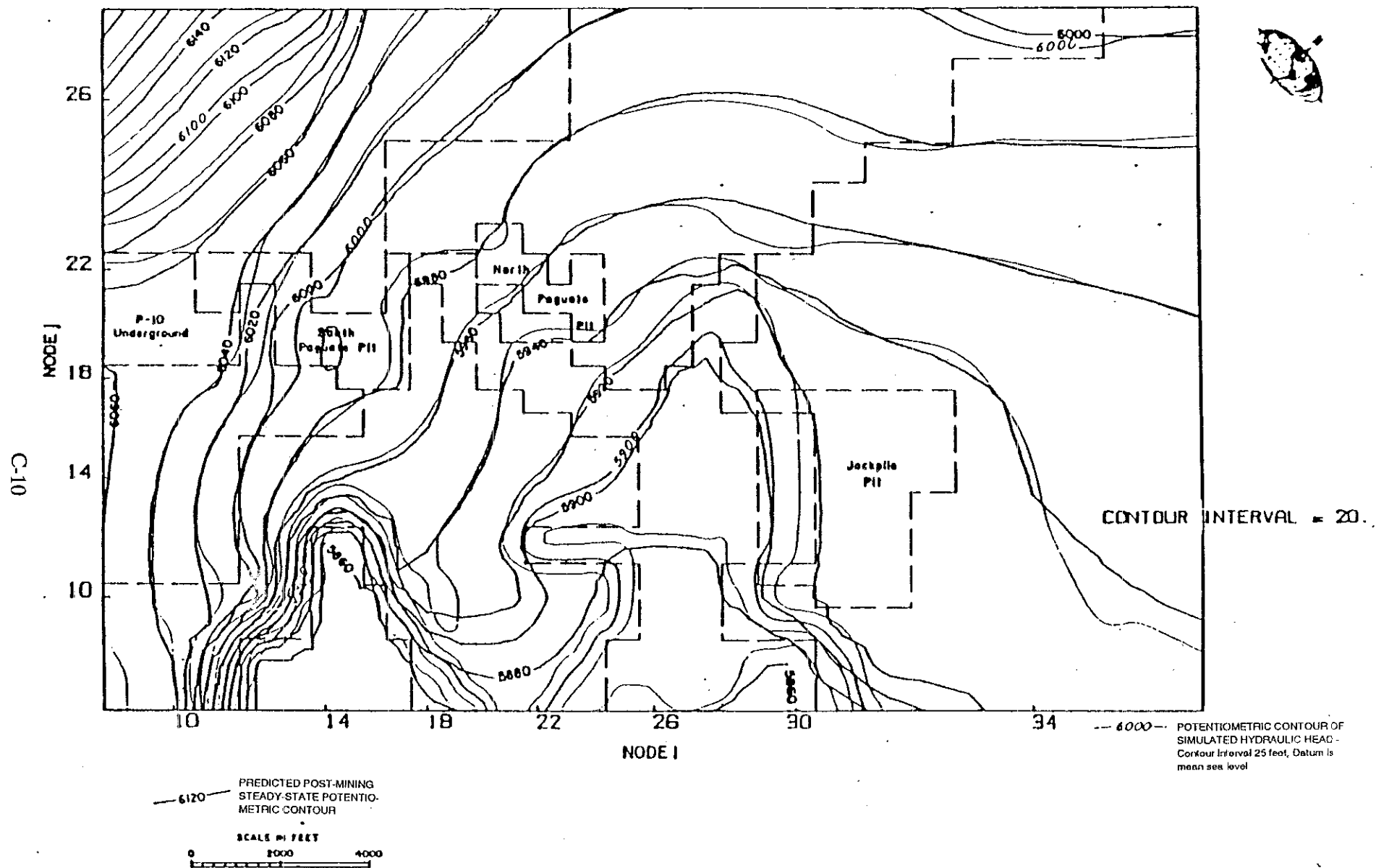


Figure C-5. Simulated post-mining and post-reclamation potentiometric heads (with artificial hydraulic barrier in the North Paguate pit) in the immediate mine area for Case 3.5.

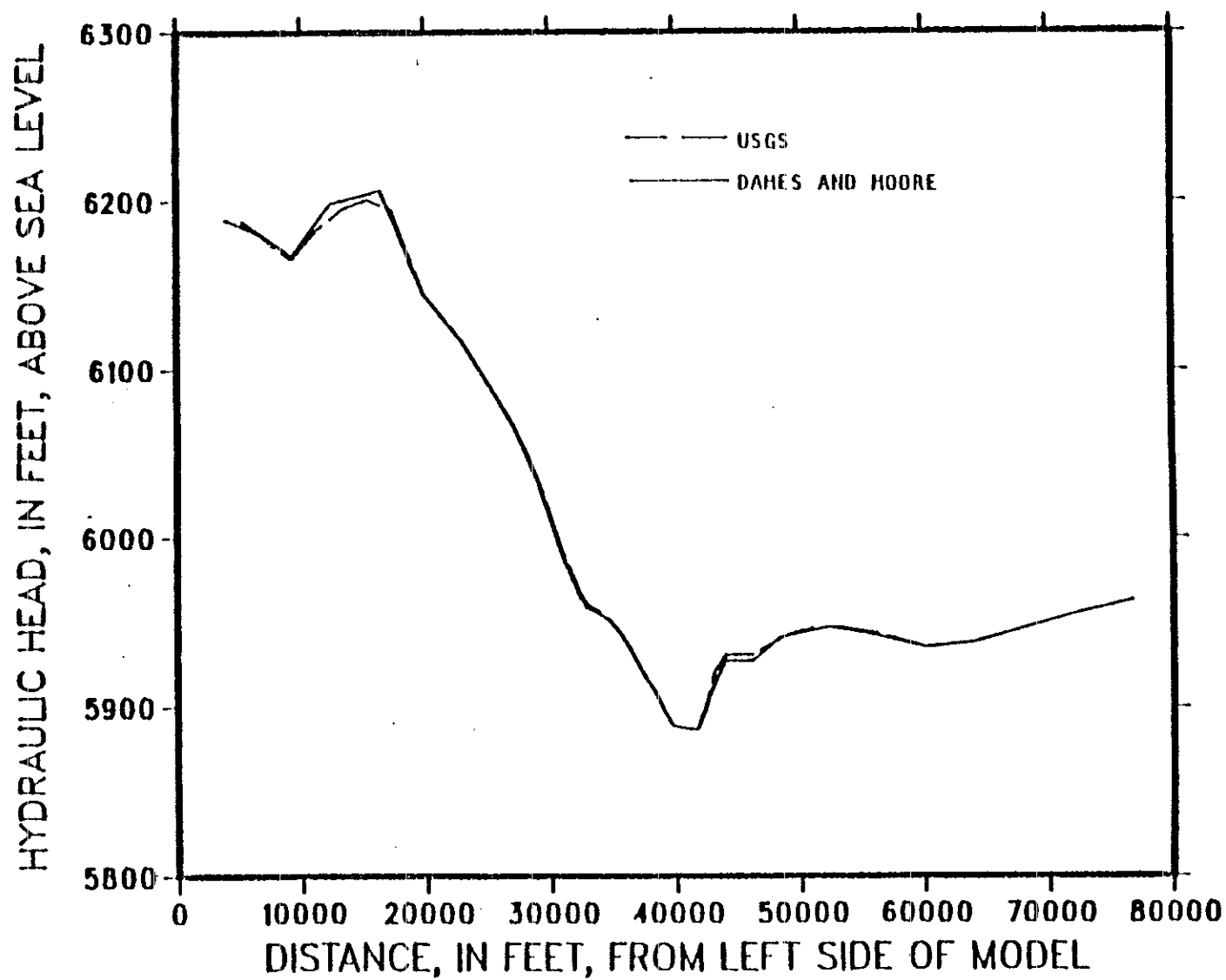


Figure C-6. Cross section of the entire modeled area along Dames & Moore model row 14 (USGS model row 28) through the Jackpile mine showing post-reclamation hydraulic heads for Case 3.5.

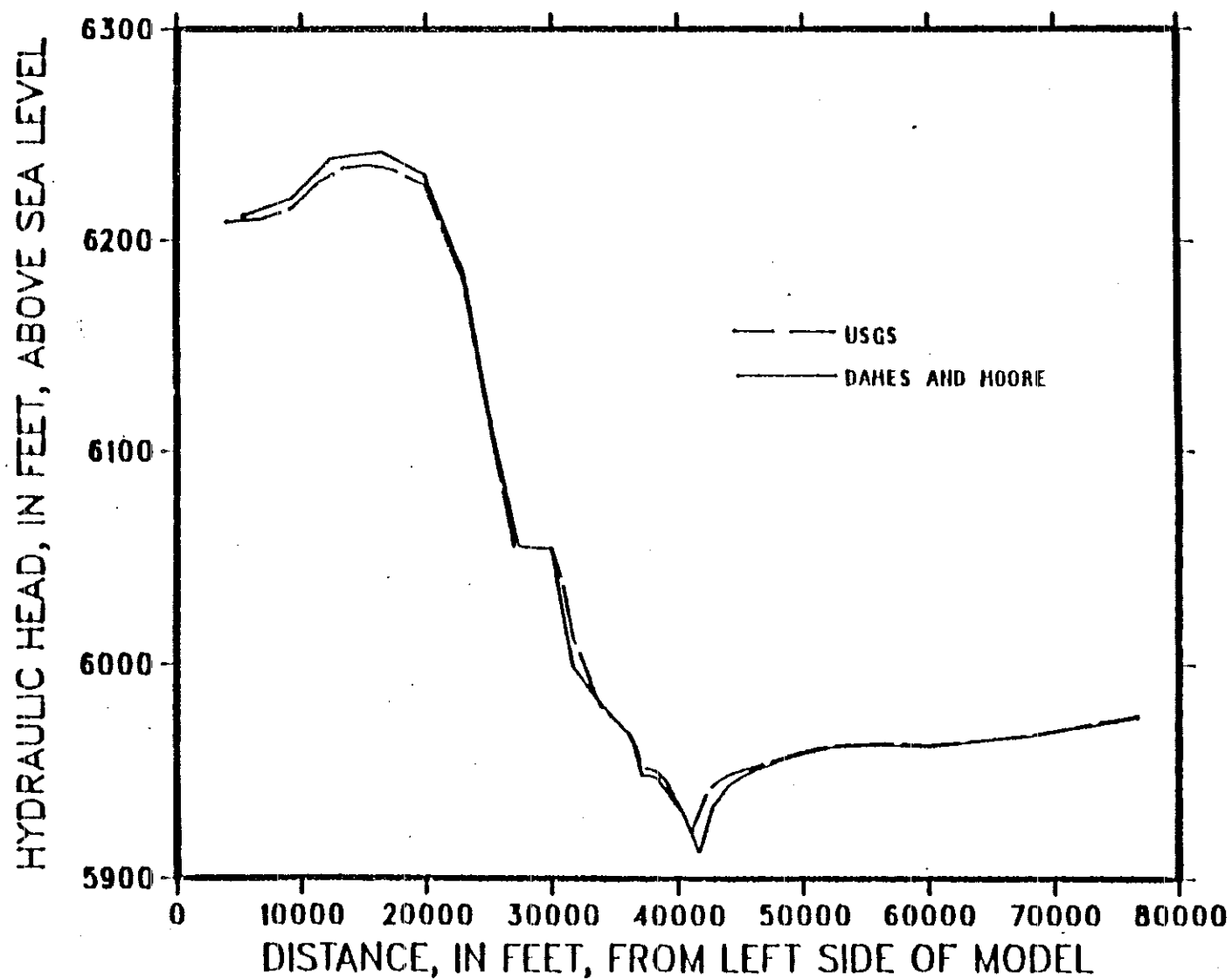


Figure C-7. Cross section of the entire modeled area along Dames & Moore model row 21 (USGS model row 21) through underground mine P10 and South and North Paguate mines showing post-reclamation hydraulic heads for Case 3.5.

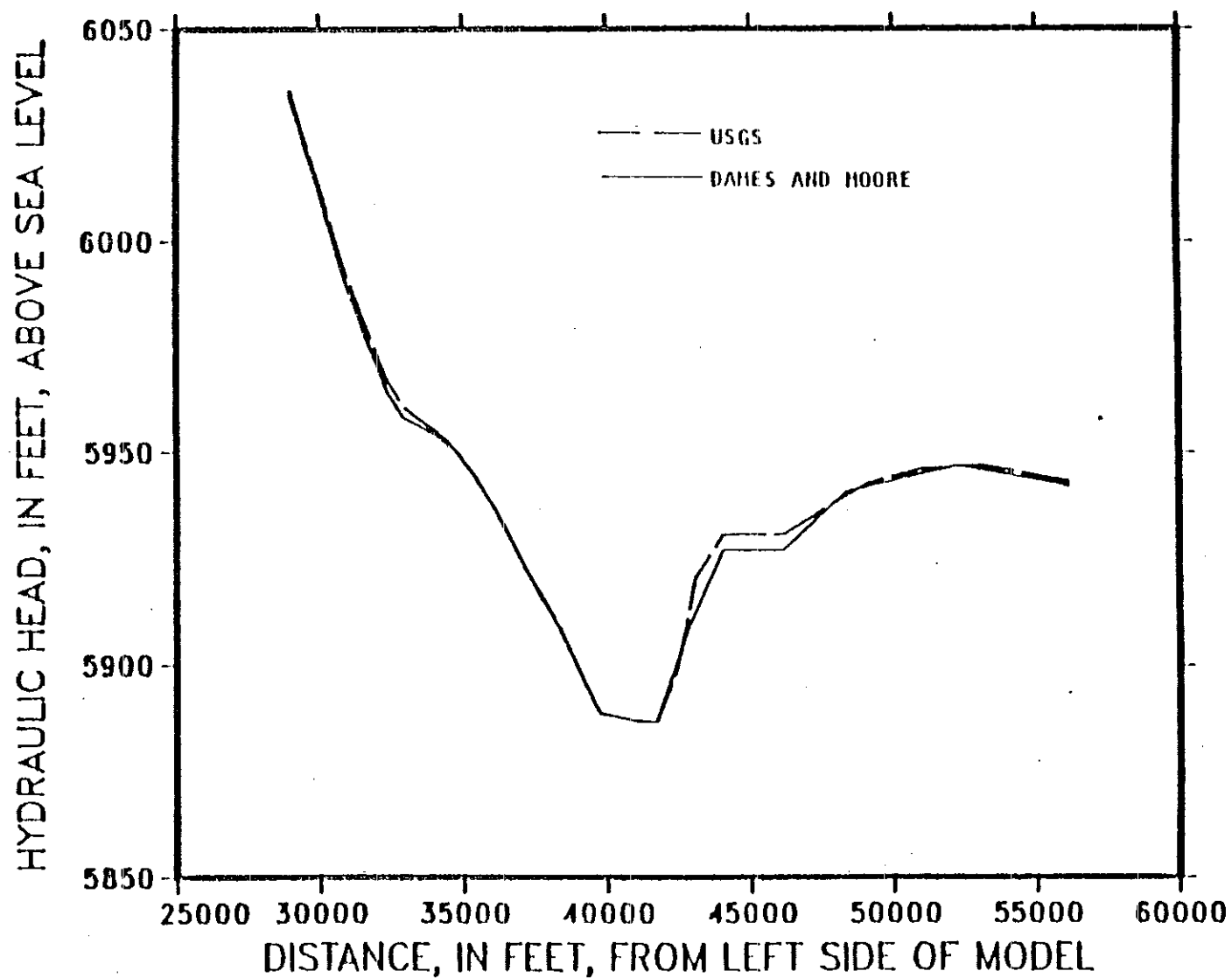


Figure C-8. Cross section of the detailed area of the model along Dames & Moore model row 14 (USGS model row 28) through the Jackpile mine showing post-reclamation hydraulic heads for Case 3.5.

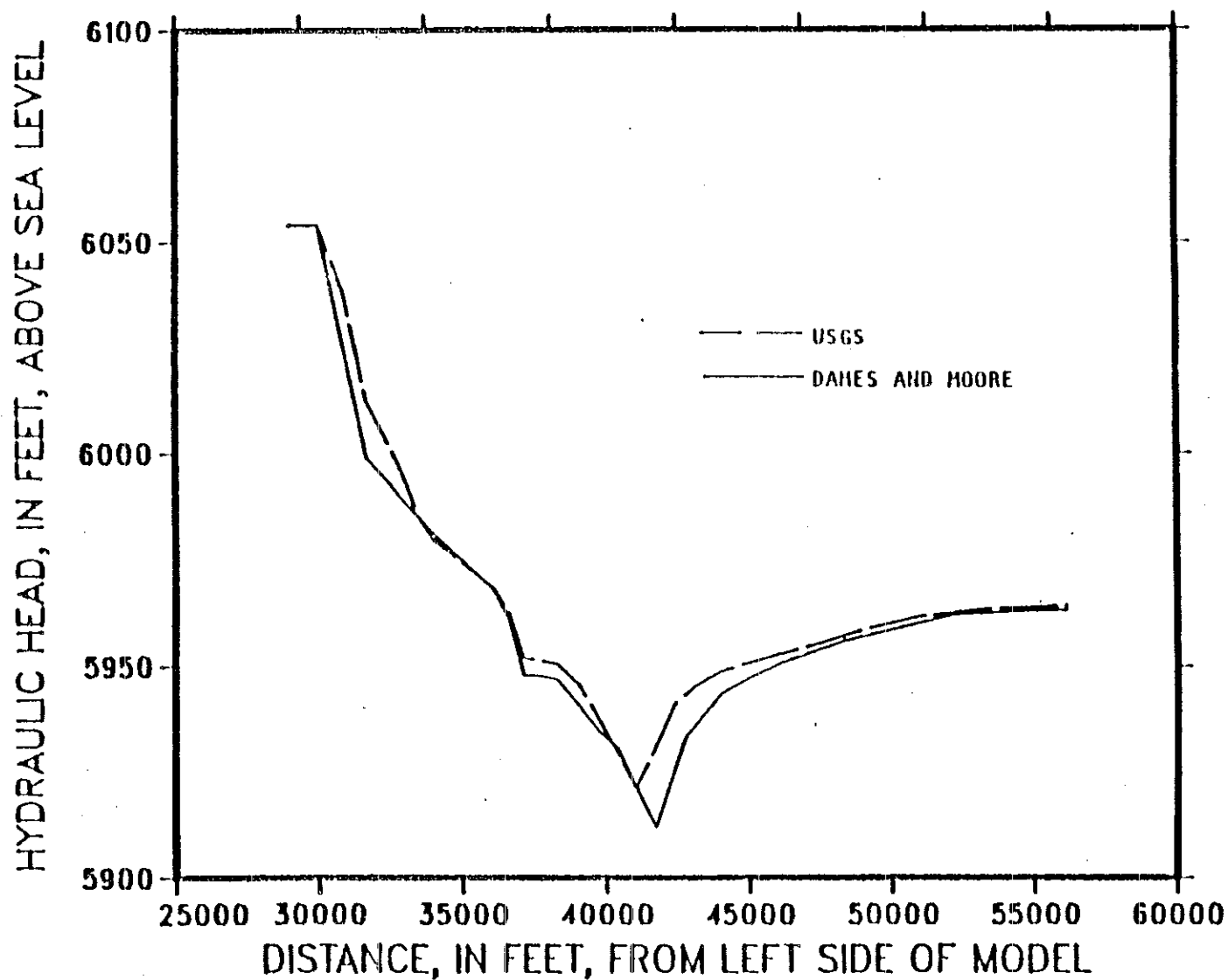


Figure C-9. Cross section of the detailed area of the model along Dames & Moore model row 21 (USGS model row 21) through underground mine P10, South and North Paguate mines showing post-reclamation hydraulic heads for Case 3.5.

CASE 8: TARGET_2DU VALIDATION—COMPARISON WITH NUMERICAL SOLUTION

Variably-Saturated Transient Flow and Transport Generated August 1987

Objective

This case illustrates the variably-saturated flow and transport capabilities of the TARGET model through application to a transient tile-drain problem analyzed by Pickens et al. (1979).

Description

Movement of water and solutes in tile-drained soils are investigated in this example application. Since the vertical planes at the tile drains and midway between tile drains are planes of symmetry, they are taken as the boundary of the calculation domain. The soil is assumed to be initially fully saturated, with the top 10 cm of soil containing contaminated water. The variation of pore pressures, location of the water table, and concentration distributions are calculated and illustrated.

Specification

The calculation domain is 5 m wide by 1.5 m deep. The tile drain is located at a depth of 0.75 m on the right-hand boundary (Figure C-10). The initial conditions for flow are hydrostatic and fully saturated. The boundary conditions for flow are zero flow on all boundaries and zero pressure head at the tile drain. Initially, the top 10 cm of soil is assumed to contain water with a solute concentration of 1.0. The lower 1.4 m of soil is assumed to contain clean water. The boundary conditions for solute transport are zero flow on all boundaries except at the tile drain.

Other soil and contaminant properties supplied to the model include

$$K = \text{saturated hydraulic conductivity} = 0.35 \text{ cm/min}$$

$$\theta_s = \text{porosity} = 0.3$$

$$S_s = \text{specific storativity} = 1 \times 10^{-5} \text{ cm}^{-1}$$

$$\left. \begin{matrix} \theta_o \\ \psi_m \\ \theta_r \\ k \\ \epsilon \end{matrix} \right\} = \text{degree of saturation parameters} = \left\{ \begin{matrix} 0.3 \\ -38.71 \text{ cm} \\ 0.09 \\ -2.85 \\ 0 \end{matrix} \right.$$

$$\left. \begin{matrix} \mu \\ \eta \end{matrix} \right\} = \text{relative hydraulic conductivity parameters} = \left\{ \begin{matrix} 2.822 \text{ cm/min} \\ 5.561 \end{matrix} \right.$$

$$D_d = \text{molecular diffusion coefficient} = 7.23 \times 10^{-5} \text{ cm}^2/\text{min}$$

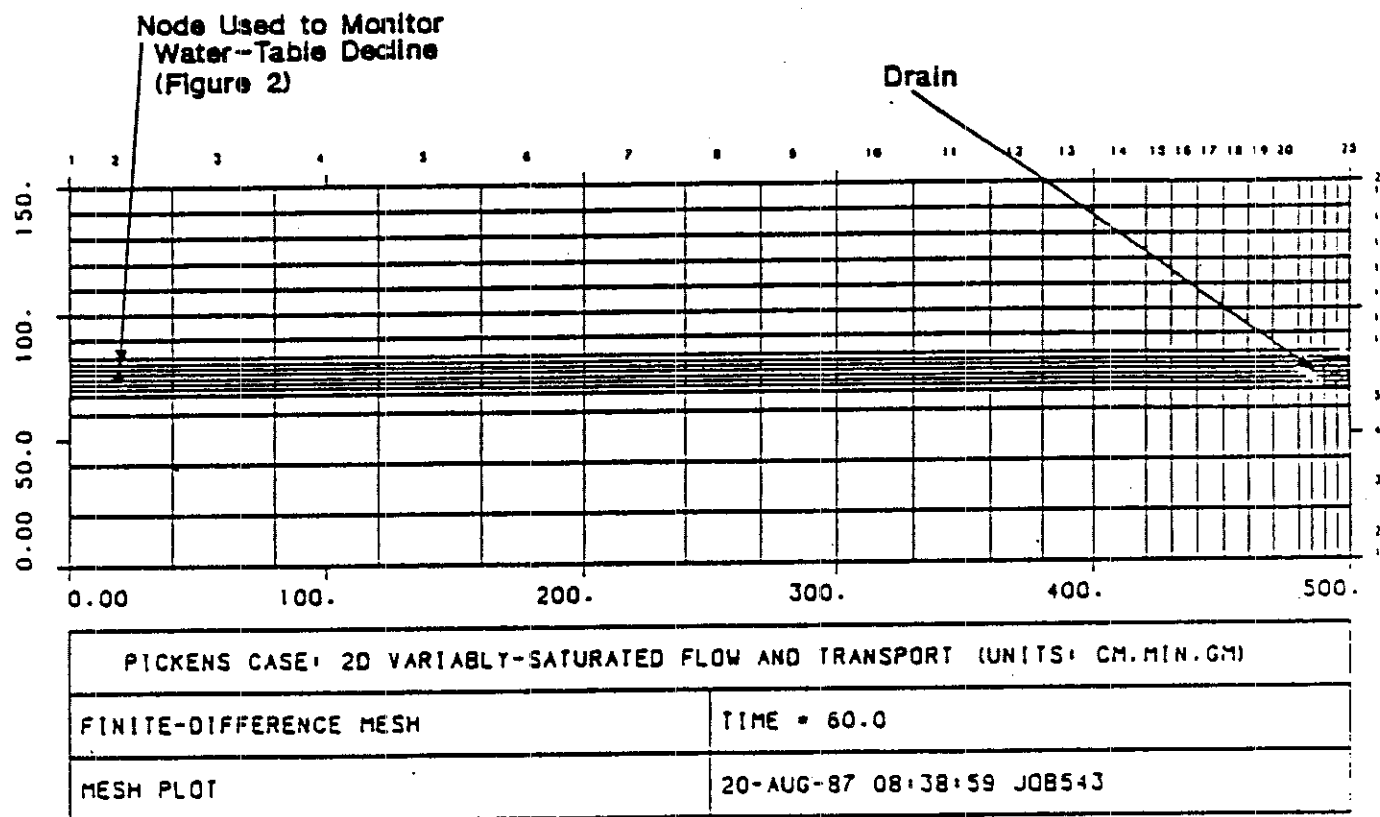


Figure C-10. Finite-difference mesh used in calculations.

D_L = longitudinal dispersivity = 2.0 cm

D_T = transverse dispersivity = 0.4 cm.

The unsaturated soil characteristic relationships describing the variation of degree of saturation (S_r) and hydraulic conductivity (K) with negative pressure heads (ψ) were taken from Pickens et al. (1979).

$$S_r(\psi) = \frac{\theta_o \left[\cosh(\psi/\psi_m)^K + \epsilon \right] - \sigma}{\theta_o \left[\cosh(\psi/\psi_m)^K + \epsilon \right] + \sigma}$$

where

$$K(\psi) = \mu \theta_s^\eta S_r^\eta$$

$$\sigma = \frac{\theta_o - \theta_r}{\theta_o + \theta_r} \cosh \epsilon$$

The finite difference calculation mesh used to discretize the domain is illustrated in Figure C-10. It consists of 25 cells in the horizontal direction, ranging in width from 5 cm to 40 cm, and 20 cells in the vertical direction, ranging in depth from 2 cm to 20 cm, for a total of 500 cells.

Results

The predicted decline of the water table is rapid at early times and more gradual as time progresses. Predicted results are illustrated in terms of hydraulic head (Figure C-11) and water-table elevations (Figure C-12) for various times up to 12 hours. The TARGET results match those obtained by Pickens et al. (1979) very closely except at early times at greater distances from the drain.

The predicted relative concentration distributions after 1 hour and 12 hours are shown in Figure C-13. The solute front moves gradually into underlying soil layers in response to the drain. The TARGET results match those obtained by Pickens et al. (1979) well except in the immediate vicinity of the drain.

Discussion

Minor variations between the TARGET and results and Pickens et al. (1979) are to be expected because (a) the shape of the drain is different between the Pickens model and the TARGET finite-difference grid, and (b) more calculation nodes were used by Pickens et al. (1979).

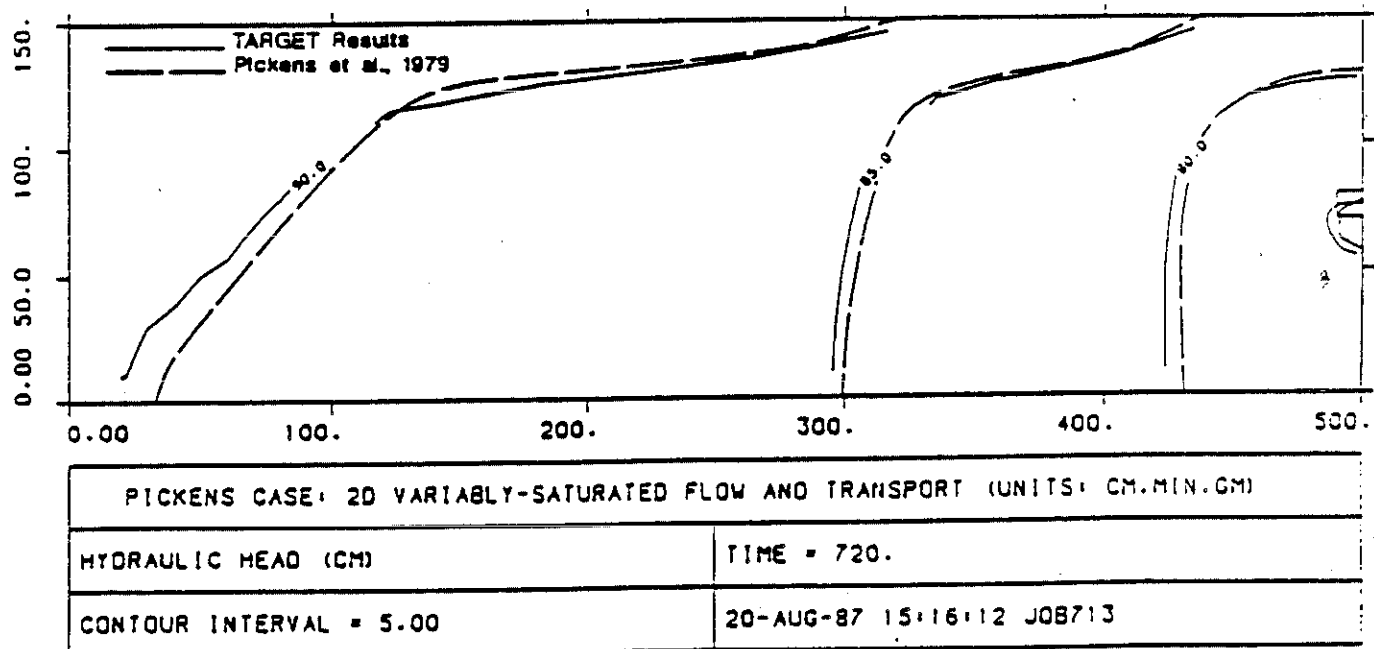
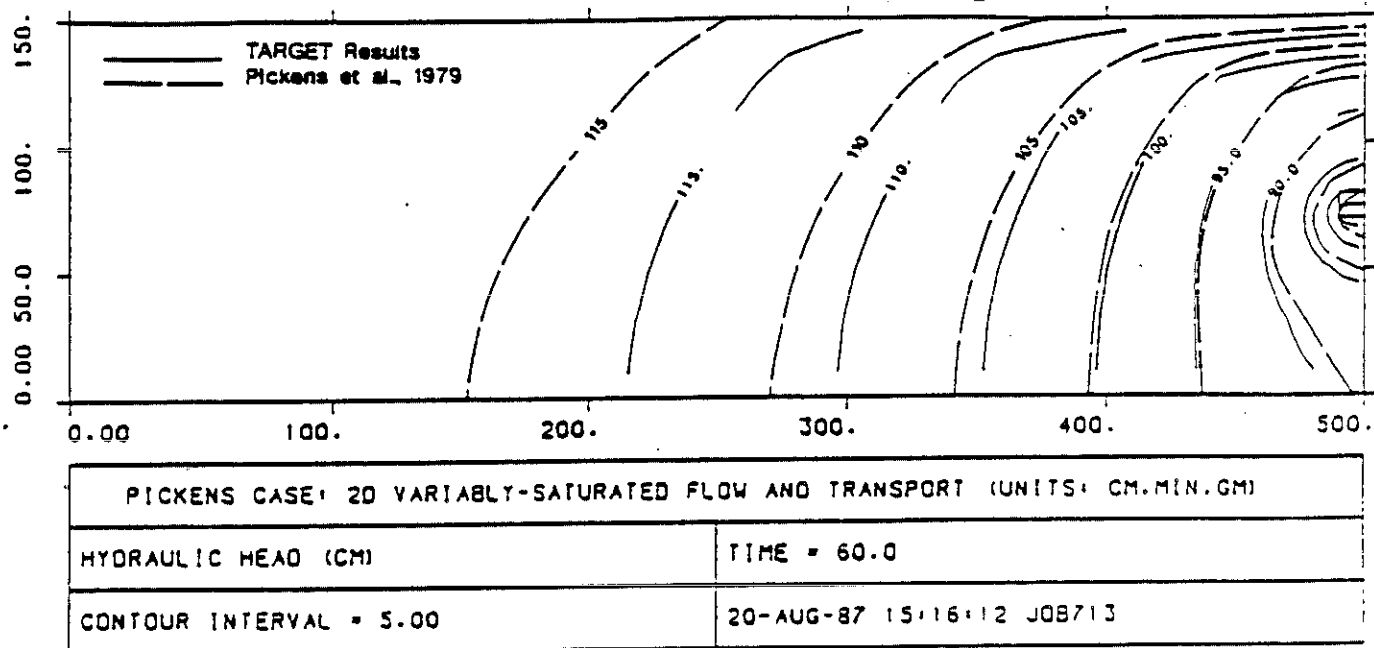
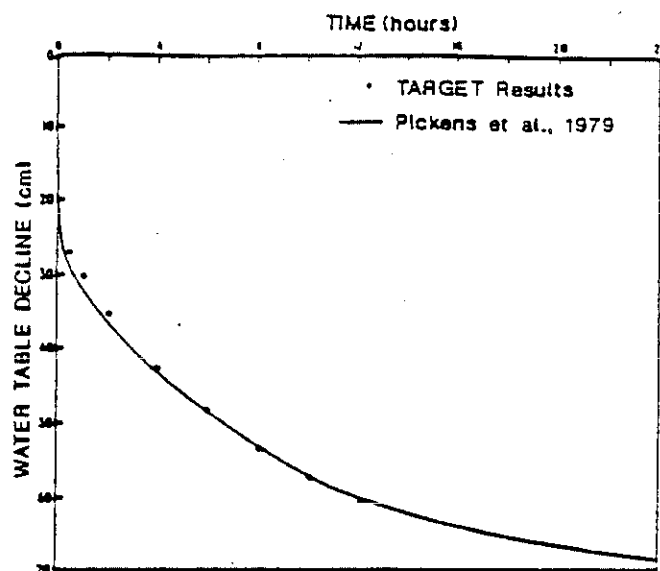


Figure C-11. Predicted hydraulic heads after 1 hour and 12 hours.



Water-table decline at the point midway between tile lines.

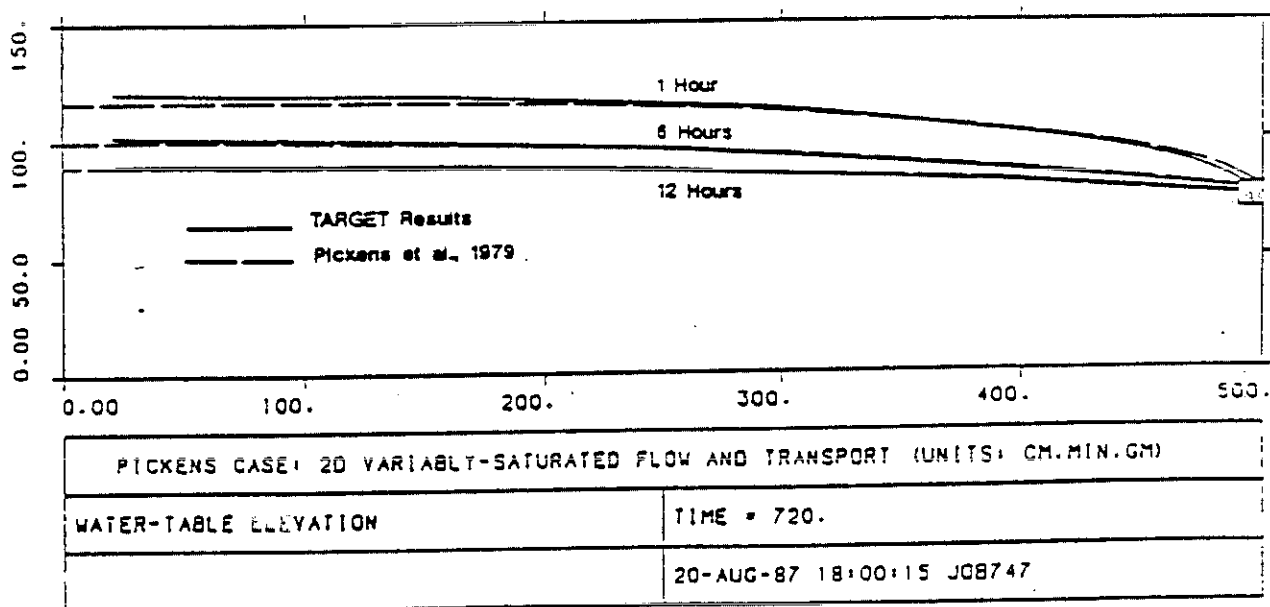
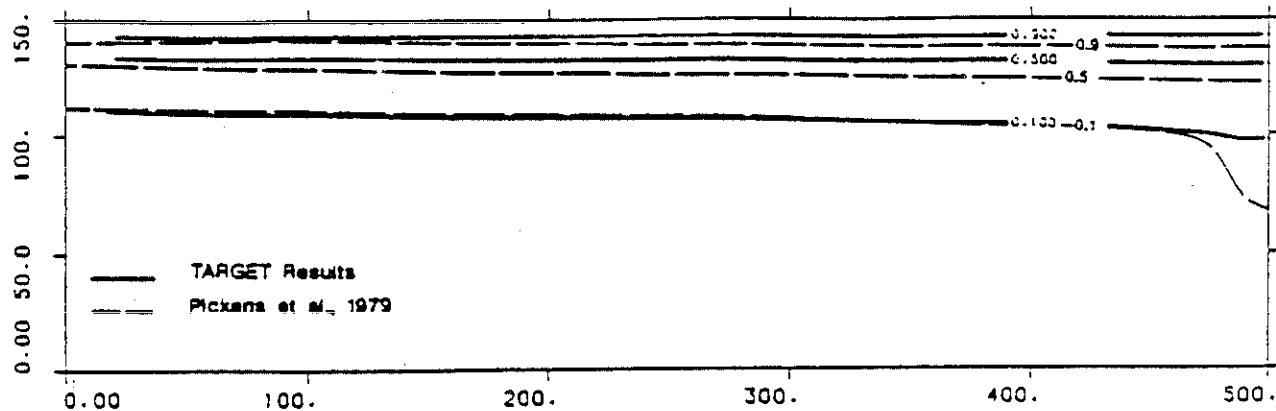
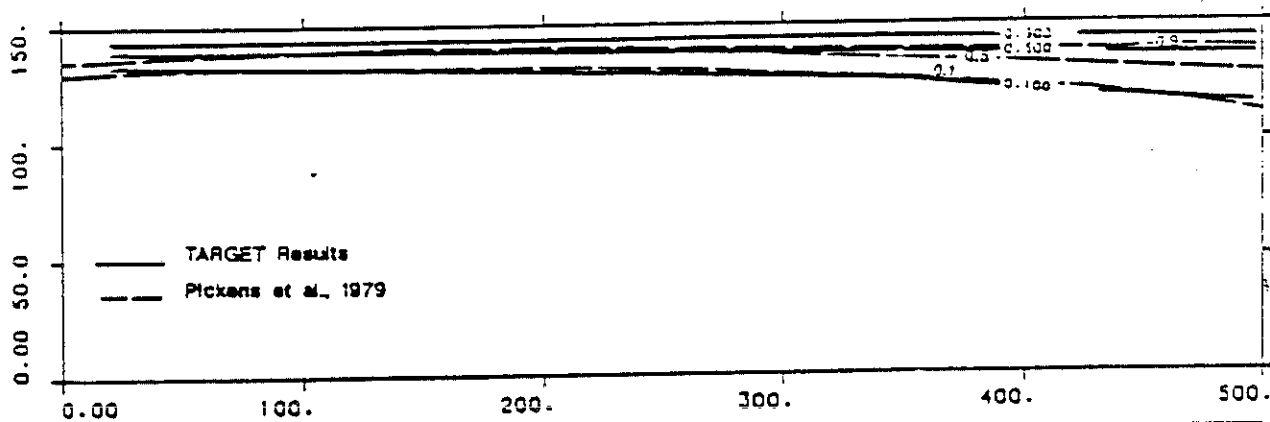


Figure C-12. Predicted water-table elevations.



PICKENS CASE: 2D VARIABLY-SATURATED FLOW AND TRANSPORT (UNITS: CM.MIN.GM)	
RELATIVE CONCENTRATION	TIME = 720.
	21-AUG-87 12:45:58 JOB1006



PICKENS CASE: 2D VARIABLY-SATURATED FLOW AND TRANSPORT (UNITS: CM.MIN.GM)	
RELATIVE CONCENTRATION	TIME = 60.0
	21-AUG-87 12:45:58 JOB1006

Figure C-13. Predicted relative concentration after 1 hour and 12 hours.

Reference

Pickens, J. F., R. W. Gaillham, and D. R. Cameron, 1979, "Finite-Element Analysis of the Transport of Water and Solutes in Tile-Drained Soils," *Journal of Hydrology*, 40, pp. 243-264.

CASE 10: TARGET_2DU AND TARGET_3DS VALIDATION COMPARISON WITH ANALYTICAL SOLUTION

Henry's Problem of Saltwater Intrusion Generated September 1987

Objective

This case simulates the movement of a saltwater wedge and compares the predicted results with analytical and numerical solutions to the same problem. The chloride concentration contours, hydraulic head distribution, and velocity vectors are plotted and compared with other solutions. This problem was simulated with both two-dimensional and three-dimensional versions of the TARGET code. The primary model feature validated in this comparison is the density-coupling of the flow and transport calculations.

Description

The situation under investigation is saltwater intrusion on a confined, freshwater aquifer; this case is known as Henry's problem (Henry 1964). Uniform freshwater flow in the confined aquifer is maintained by uniform inflow at the upgradient edge of the domain. The downgradient edge of the domain is at the coast, in contact with saltwater of higher density than the freshwater. The saltwater wedge that develops under equilibrium conditions is investigated.

Specification

The specifications for this problem were selected to match the cases analyzed by others (Pinder and Cooper 1970, Lee and Cheng 1974, Segol and Pinder 1976, Frind 1982, Huyakorn et al. 1984, Huyakorn et al. 1987). Uniform freshwater inflow occurs into a confined, coastal aquifer of uniform width and depth. The aquifer dimensions and boundary conditions are summarized in Figure C-14.

The model simulation used a finite-difference grid with 16 cells in the horizontal direction and 11 cells in the vertical direction. The calculation cells ranged in size from 10 m by 10 m to 10 m by 20 m, with the smaller cells concentrated in the area of saltwater intrusion.

Zero heads and concentrations were assumed as initial conditions. Other parameters supplied to the model included the following:

x-direction hydraulic conductivity	=	1 m/s
z direction hydraulic conductivity	=	1 m/s
porosity	=	0.35
longitudinal and transverse dispersivity	=	0.0
molecular diffusion coefficient	=	$6.6 \times 10^{-2} \text{ m}^2/\text{s}$

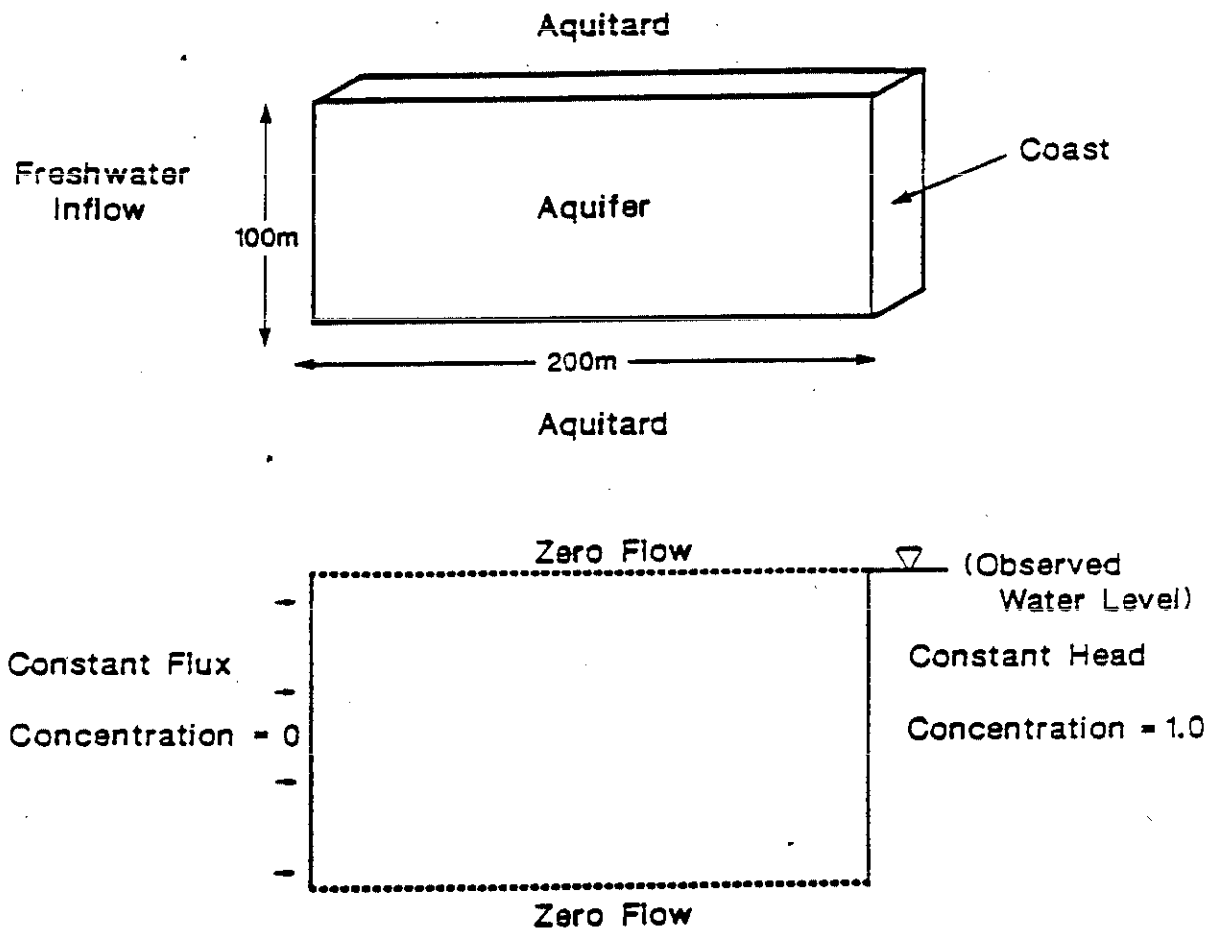


Figure C-14. Schematic representation of Henry's Problem.

tortuosity	=	0.35
freshwater influx	=	6.6×10^{-3} m/s
density difference ratio	=	0.025

Results

The model predictions and numerical and (where available) analytical solutions for the equilibrium isochlors, hydraulic head distribution, and velocity vectors are shown in Figures C-15 through C-17, respectively. The figures show that the predictions by the present method are in good agreement with those presented by other authors.

Discussion

The portion of the coastal interface that becomes an outflow boundary has been treated differently by various authors, with resulting variations in the predicted results. In the present method, fixed concentration boundaries are automatically reset to zero gradient concentration boundaries along advection-dominated outflow segments of the boundary. This is a modification to the boundary conditions used in the original analytical solution (Henry 1959), but is a more realistic representation of the physical problem used by later workers (e.g., Huyakorn 1987).

References

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- Henry, H. R., 1959, "Salt Intrusion into Freshwater Aquifers," *Journal of Geophysical Research*, 64, pp. 1911-1919.
- Henry, H. R., 1964, "Effects of Dispersion on Salt Encroachment in Coastal Aquifers," *U.S. Geological Survey Water Supply Paper 1613-C*.
- Huyakorn, P. S., J. W. Mercer, and P. F. Andersen, 1984, *SWICHA: A Three-Dimensional Finite Element Code for Analyzing Seawater Intrusion in Coastal Aquifers*.
- Huyakorn, P. S., P. F. Andersen, J. W. Mercer, and H. O. White, Jr., 1987, "Saltwater Intrusion in Aquifers: Development and Testing of a Three-Dimensional Finite Element Model," *Water Resources Research*, 23, 1, pp. 293-312.
- Lee, C. H., and R. T. Cheng, 1976, "On Seawater Encroachment in Coastal Aquifers," *Water Resources Research*, 10, 5, pp. 1039-1043.
- Pinder, G. F., and H. H. Cooper, Jr., 1970, "A Numerical Technique for Calculating the Transient Position of the Saltwater Front," *Water Resources Research*, 6, 3, pp. 875-880.
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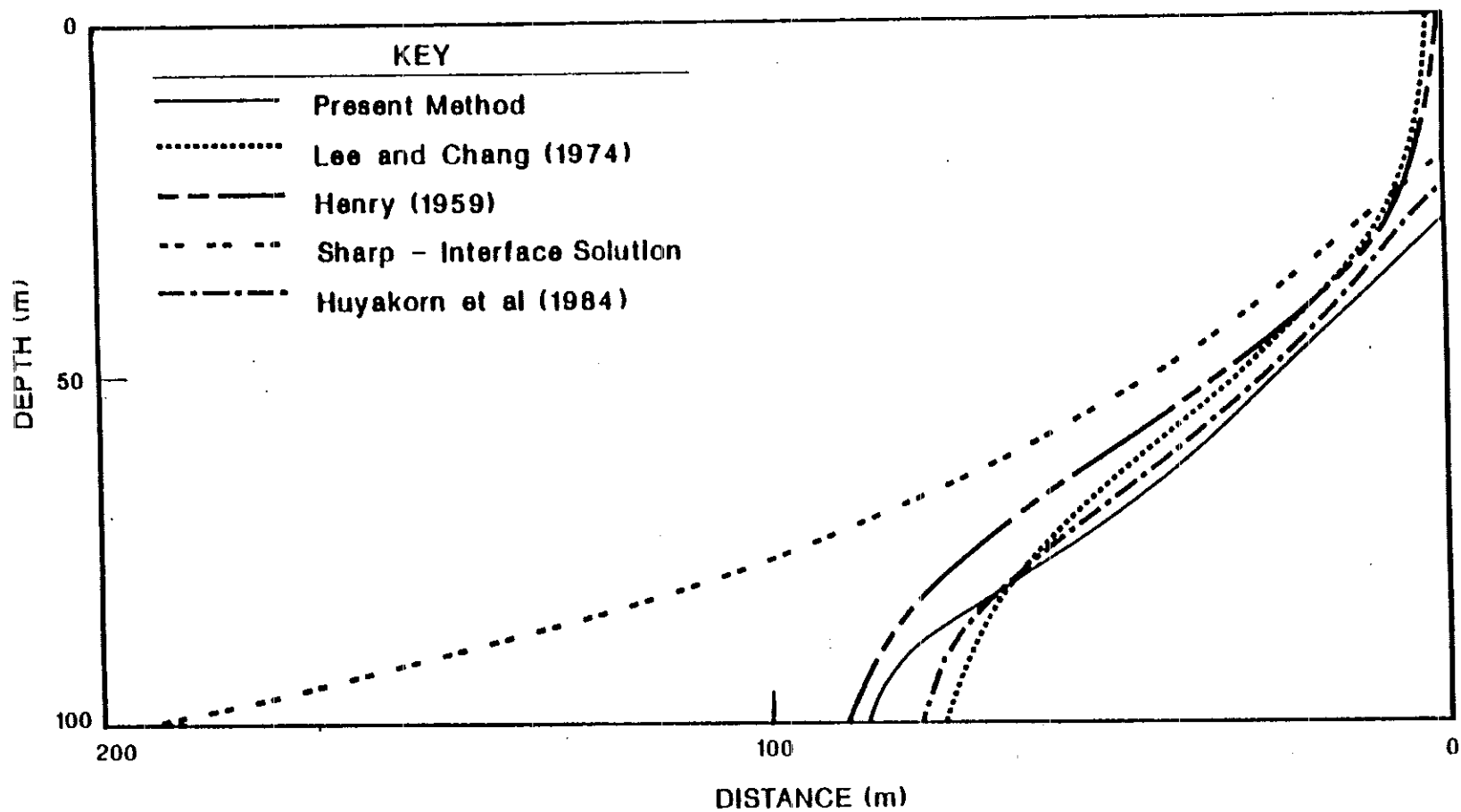


Figure C-15. Predicted 0.5 isochlors for Henry's Problem.

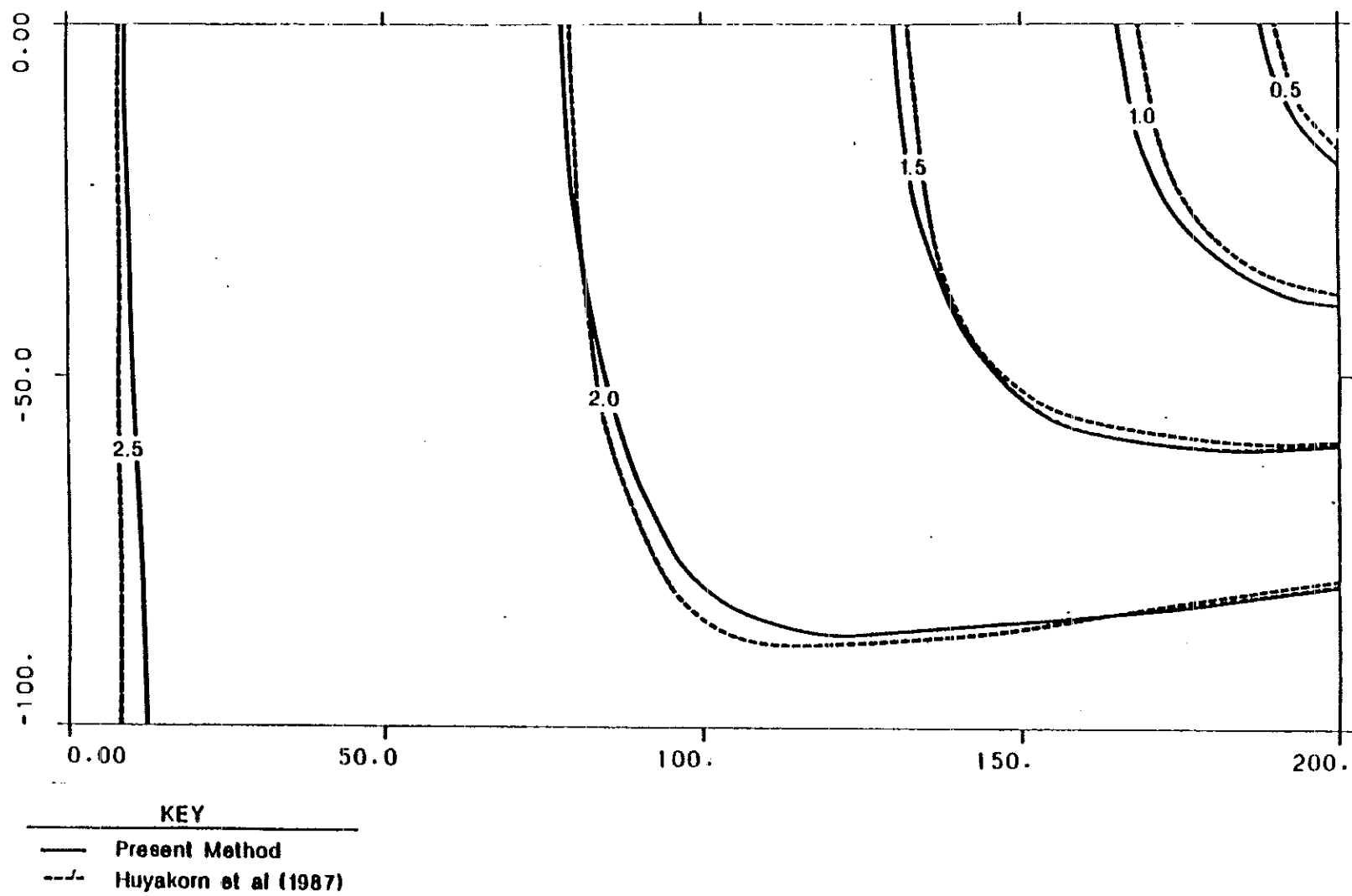
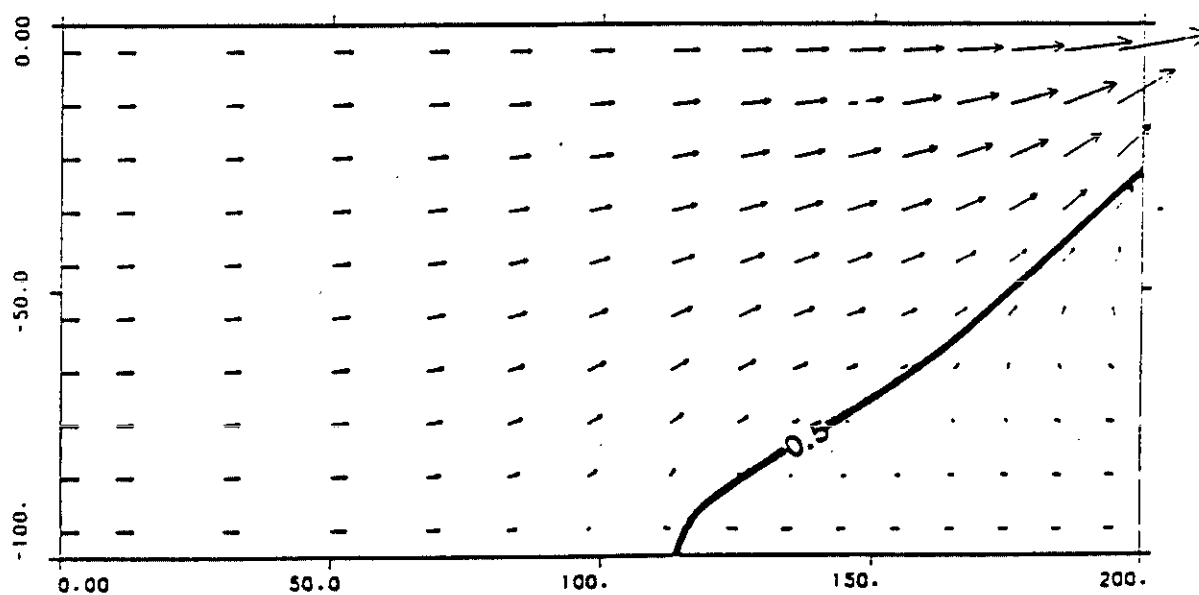
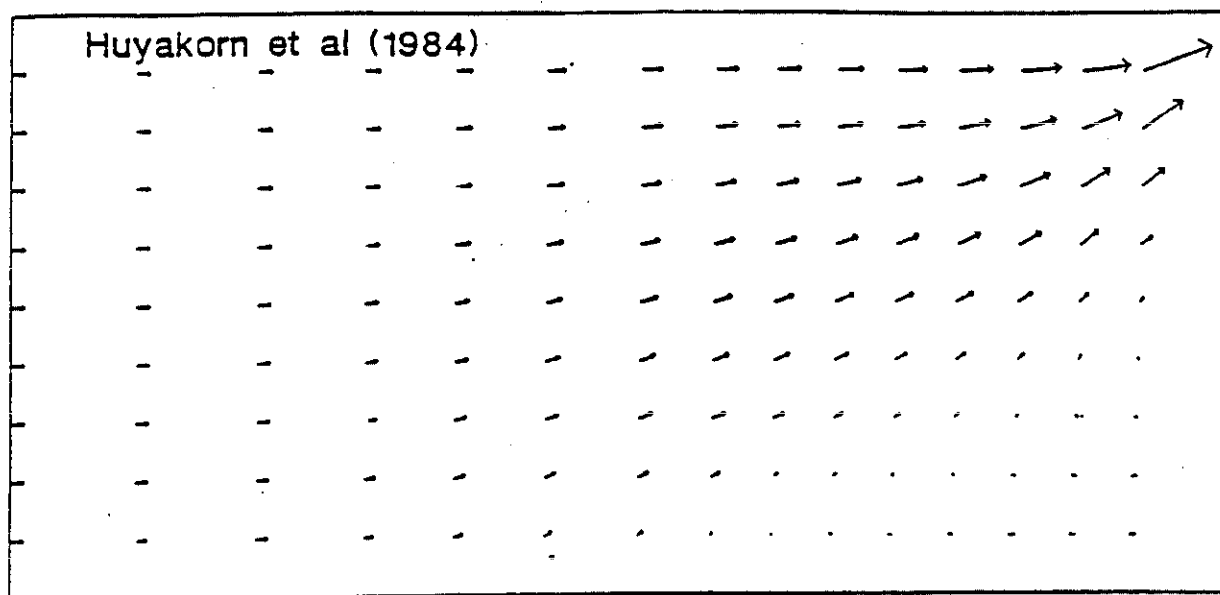


Figure C-16. Steady-state reference hydraulic head distribution.



HENRY'S PROBLEM OF 2D SEAWATER INTRUSION IN CONFINED AQUIFER (UNITS: FCS)	
FLUX VECTORS	Results of Present Method
→ = 0.0403	18-AUG-87 12:35:39 JOB15

Figure C-17. Steady-state velocity field for Henry's Problem.

Appendix D

List of Publications on the TARGET Models

Appendix D

List of Publications on the TARGET Models

- Highland, W. R., 1984, "Limitations in Applying Mathematical Models to the Analysis of Contaminant Transport from Waste Disposal Sites," *Proceedings of NWWA Conference on Practical Applications of Ground-Water Models, Columbus, Ohio.*
- Highland, W. R., P. J. Pralong, and D. Sharma, 1983, "Evaluation and Management of Ground-Water Contamination With Mathematical Modeling," *Proceedings of International Conference on Ground Water and Man, Sydney, Australia.*
- Highland, W. R., L. T. Murdock, and E. Kemp, 1981, "Design and Seepage Modeling Studies of Below-Grade Disposal, West Gas Hills, Wyoming," *Proceedings of Symposium on Uranium Mill Tailings Management, Fort Collins, Colorado.*
- Moreno, J. L., and S. A. Moreno, 1987, "A Three-Dimensional Mathematical Model of Contaminant Transport for Microcomputers," *Proceedings of Geotech 1987, Denver, Colorado.*
- Moreno, J. L., 1989, "Three-Dimensional Simulation of the Migration and Cleanup of Trichloroethylene," *Proceedings of Fourth International Conference, Solving Ground-Water Problems with Models, Indianapolis, Indiana.*
- Moreno, J. L., and R. D. Bartlett, 1987, "Ground-Water Model Planning: The Limitations of Data," *Proceedings of Waste Management Conference: Focus on The West, Fort Collins, Colorado.*
- Sharma, D., 1981, "Some Applications of a Novel Computational Procedure for Solving the Richards Equation," *Proceedings of AGU Fall Meeting, San Francisco, California.*
- Sharma, D., J. L. Moreno, and M. I. Asgian, 1981, "A Computational Procedure for Predicting Coupled Fluid Flows and Transport of Reactive Chemical Species in Variably-Saturated Porous Media," *Joint ASME/ASCE Mechanics Conference, Boulder, Colorado.*
- Sharma, D., P. J. Pralong, 1982, "Transient Freezing and Thawing Around Buried Pipelines," *Proceedings of International Symposium on Numerical Methods in Geomechanics, Zurich, Switzerland.*
- Sharma, D., 1982, "Fluid Dynamics and Mass Transfer in Variably-Saturated Porous Media: Formulation and Applications of a Mathematical Model," *Battelle-NRC Symposium, Seattle, Washington.*
- Sharma, D., M. I. Asgian, W. R. Highland, and J. L. Moreno, 1983, "Analysis of Complex Seepage Problems with the Disposal of Uranium Tailings: Selected Case Studies," *Mineral and Energy Resources*, 26, 1.